```
=> d his ful

     (FILE 'HOME' ENTERED AT 08:54:18 ON 20 AUG 2005)

     FILE 'REGISTRY' ENTERED AT 08:54:23 ON 20 AUG 2005
L2             STR
L3          120699 SEA SSS FUL L2
L4             STR
L5           51757 SEA SUB=L3 SSS FUL L4
L9             STR
L10            STR L9
L11            STR
L12            STR L9
L13            STR L12
L17            STR L15
L20           1437 SEA SSS FUL L9 OR L10 OR L11 OR L12 OR L13
L21            STR L17
L22            210 SEA SSS FUL L17
L23            STR L15
L24              9 SEA SUB=L22 SSS FUL L23

     FILE 'HCAPLUS' ENTERED AT 09:22:38 ON 20 AUG 2005
L25            484 SEA ABB=ON  PLU=ON  L24
L26          15691 SEA ABB=ON  PLU=ON  L5
L27           8894 SEA ABB=ON  PLU=ON  L20
L28              2 SEA ABB=ON  PLU=ON  L25 AND L26 AND L27
                 D STAT QUE
                 D IBIB ABS HITSTR L28 1-2
L32             89 SEA ABB=ON  PLU=ON  L26 AND L27
L36             27 SEA ABB=ON  PLU=ON  L24/P
L37             14 SEA ABB=ON  PLU=ON  L25 AND L26
L38             12 SEA ABB=ON  PLU=ON  L25 AND L27
L39             70 SEA ABB=ON  PLU=ON  L32 AND PD=<OCTOBER 9, 2002
L40             39 SEA ABB=ON  PLU=ON  L36 OR L37 OR L38
L41             14 SEA ABB=ON  PLU=ON  L40 AND PD=<OCTOBER 9, 2002
                 D IBIB ABS HITSTR L41 1-14
L42             70 SEA ABB=ON  PLU=ON  L39 NOT (L41 OR L28)
L45           3967 SEA ABB=ON  PLU=ON  L26(L)REACTANT/RL
L46           6032 SEA ABB=ON  PLU=ON  L27(L)REACTANT/RL
L47             32 SEA ABB=ON  PLU=ON  (L45 AND L46) AND L42
                 D STAT QUE
                 D IBIB ABS HITSTR L47 1-32


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   19 AUG 2005  HIGHEST RN 861198-35-8
     DICTIONARY FILE UPDATES:  19 AUG 2005  HIGHEST RN 861198-35-8

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

       Please note that search-term pricing does apply when
       conducting SmartSELECT searches.
```

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**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from  *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

FILE HCAPLUS

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FILE COVERS 1907 - 20 Aug 2005  VOL 143 ISS 9
FILE LAST UPDATED: 19 Aug 2005  (20050819/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 09:22:38 ON 20 AUG 2005
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 20 Aug 2005  VOL 143 ISS 9
FILE LAST UPDATED: 19 Aug 2005  (20050819/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=>
=>

=> d stat que
L2                STR
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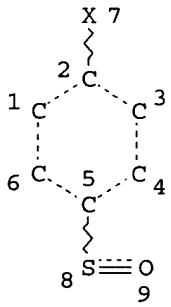


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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
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L4                STR
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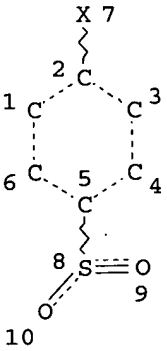

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
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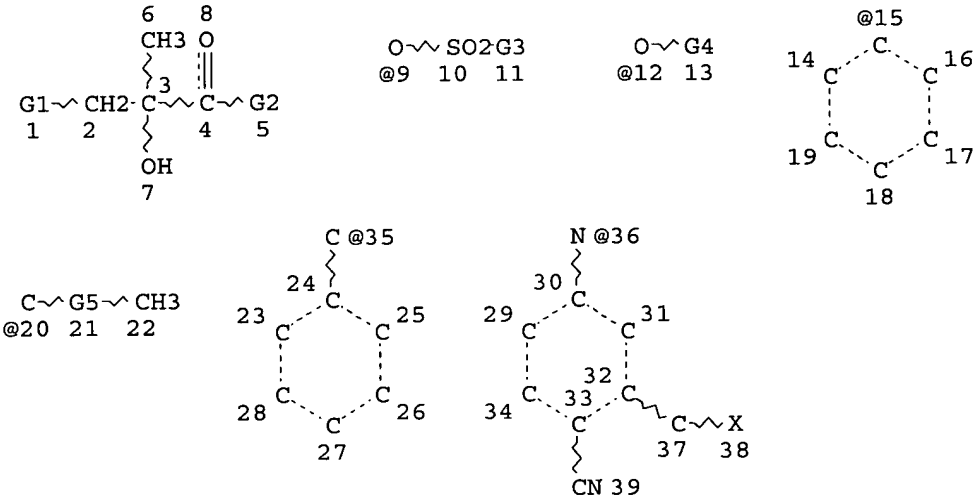
L9 STR



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VAR G4=ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/20/CB/35/36
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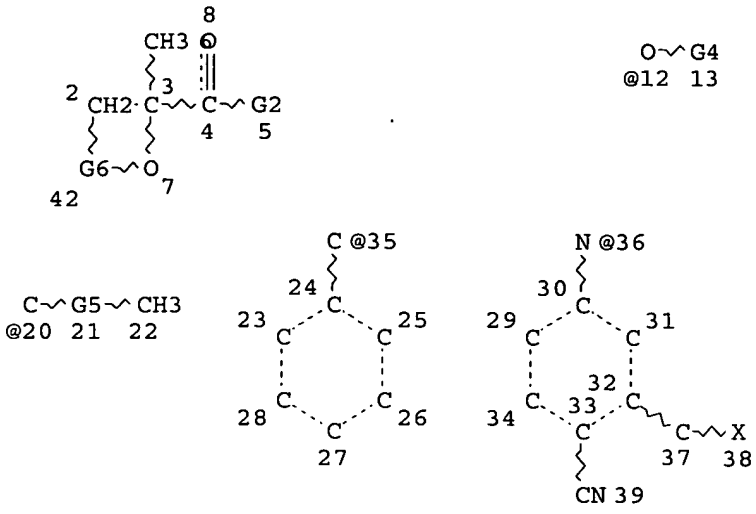
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 39

STEREO ATTRIBUTES: NONE

L10 STR



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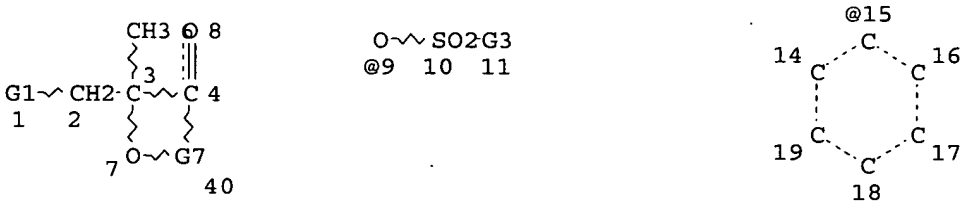
REP G6=(0-3) A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE
L11 STR



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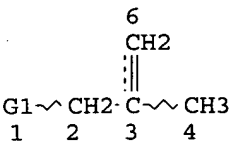
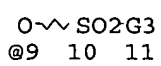
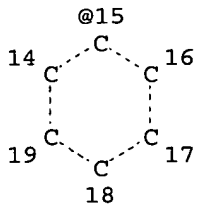
REP G7=(2-7) A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L12 STR







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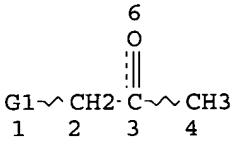
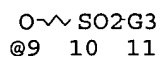
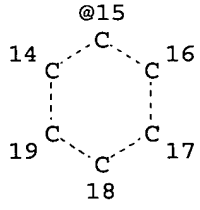
VAR G3=OH/ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/15
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L13 STR



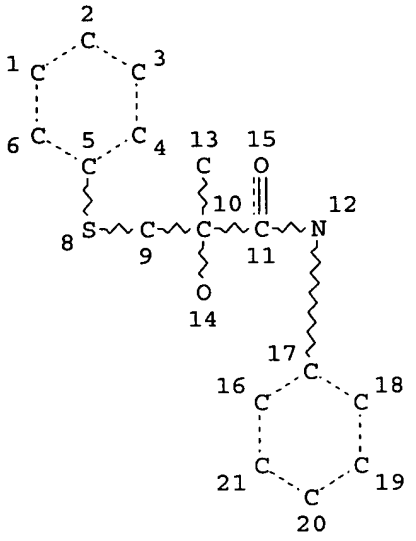




VAR G1=X/9
VAR G3=OH/ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/15
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L17 STR



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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
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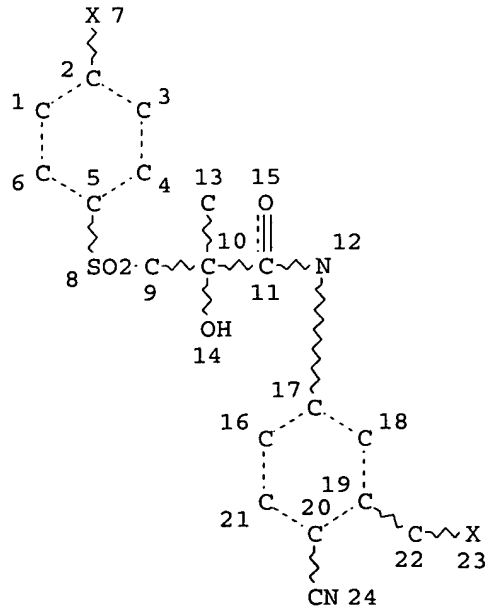
L22 210 SEA FILE=REGISTRY SSS FUL L17
L23 STR



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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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L25         484 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L24
L26       15691 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L5
L27        8894 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20
L28           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L25 AND L26 AND L27
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=>
=>

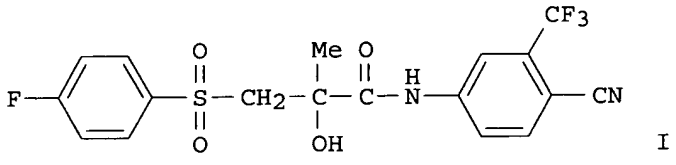
=> d ibib abs hitstr l28 1-2

L28 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	2004:293441 HCAPLUS
DOCUMENT NUMBER:	140:303414
TITLE:	Process for making bicalutamide and intermediates thereof
INVENTOR(S):	Thijs, Lambertus; Keltjens, Rolf; Ettema, Gerrit J. B.
PATENT ASSIGNEE(S):	Neth.
SOURCE:	U.S. Pat. Appl. Publ., 23 pp., Cont.-in-part of U.S. Ser. No. 261,492. CODEN: USXXCO
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004068135	A1	20040408	US 2003-682530	20031010
US 2003073742	A1	20030417	US 2002-261492	20021002
US 6818766	B2	20041116		
PRIORITY APPLN. INFO.:			US 2002-261492 A2	20021002
OTHER SOURCE(S):	MARPAT 140:303414			

GI



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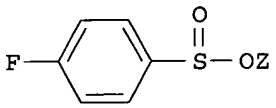


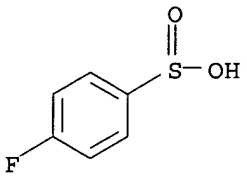
II

AB Bicalutamide (I) and/or its intermediates are made by reaction of p-fluorobenzenesulfinic acid salt (II; Z = a cation) with 2-hydroxyisobutyric acid derivs. of formula YCH2C(Me)(OX)COA (A = OR; wherein R = H, C1-6 alkyl, C3-6 cycloalkyl, Ph, benzyl,4-cyano-3-trifluoromethylanilino; Y = leaving group and X = H; or X and Y are joined together to form a 3- to 6-membered heterocyclic ring, in particular oxirane ring; or X and A are joined together to form a 5- to 10-membered fused or unfused heterocyclic ring with the proviso that if a ring nitrogen is present, it may be substituted by a 3-trifluoromethyl-4-cyanophenyl group), YCH2CMe:CH2 (Y = same as above), or YCH2COMe (Y = same as above). Thus, 0.500 g N-[4-cyano-3-(trifluoromethyl)phenyl]-2-methyl-2-oxiranecarboxamide (III) was dissolved in dissolved in a mixture of 40 mL CHCl3 and 40 mL H2O, successively treated with 371 mg sodium p-fluorobenzenesulfinate and 298 mg tetrabutylammonium bromide, and refluxed for 96 h to give, after workup and silica gel chromatog., 380 mg I (48% yield). Similarly, chiral (R)-I was obtained using chiral epoxide (S)-III in 43% yield.

IT **676559-19-6**, Ammonium p-fluorobenzenesulfinate
RL: RCT (Reactant); RACT (Reactant or reagent)
(claimed compound; preparation of bicalutamide by coupling of N-[4-cyano-3-(trifluoromethyl)phenyl]-2-methyl-2-orixanecarboxamide or -3-(halo or mesyloxy)-2-hydroxy-2-methylpropanamide with sodium p-fluorobenzenesulfinate)

RN 676559-19-6 HCAPLUS

CN Benzenesulfinic acid, 4-fluoro-, ammonium salt (9CI) (CA INDEX NAME)

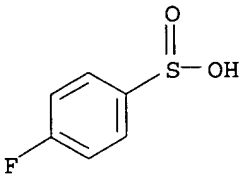


● NH_3

IT **824-80-6**, Sodium p-fluorobenzenesulfinate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bicalutamide by coupling of N-[4-cyano-3-(trifluoromethyl)phenyl]-2-methyl-2-orixanecarboxamide or -3-(halo or mesyloxy)-2-hydroxy-2-methylpropanamide with sodium p-fluorobenzenesulfinate)

RN 824-80-6 HCAPLUS

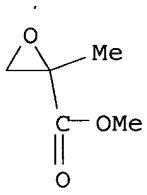
CN Benzenesulfinic acid, 4-fluoro-, sodium salt (9CI) (CA INDEX NAME)



● Na

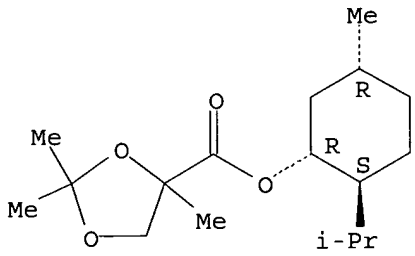
IT **58653-97-7P**, Methyl 2-methyl-2-oxiranecarboxylate
512776-89-5P, (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl 2,2,4-trimethyl-1,3-dioxolane-4-carboxylate **512776-90-8P**, Sodium 2,2,4-trimethyl-1,3-dioxolane-4-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bicalutamide by coupling of N-[4-cyano-3-(trifluoromethyl)phenyl]-2-methyl-2-orixanecarboxamide or -3-(halo or mesyloxy)-2-hydroxy-2-methylpropanamide with sodium p-fluorobenzenesulfinate)

RN 58653-97-7 HCAPLUS
CN Oxiranecarboxylic acid, 2-methyl-, methyl ester (9CI) (CA INDEX NAME)

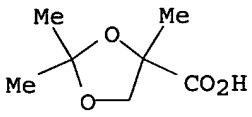


RN 512776-89-5 HCAPLUS
CN 1,3-Dioxolane-4-carboxylic acid, 2,2,4-trimethyl-, (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



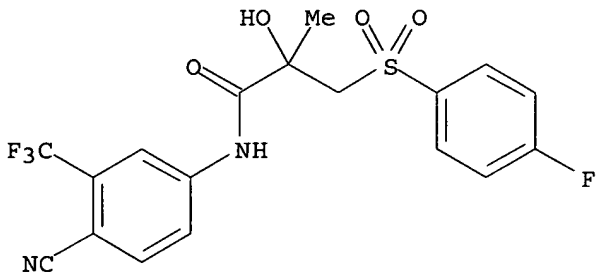
RN 512776-90-8 HCAPLUS
CN 1,3-Dioxolane-4-carboxylic acid, 2,2,4-trimethyl-, sodium salt (9CI) (CA INDEX NAME)



● Na

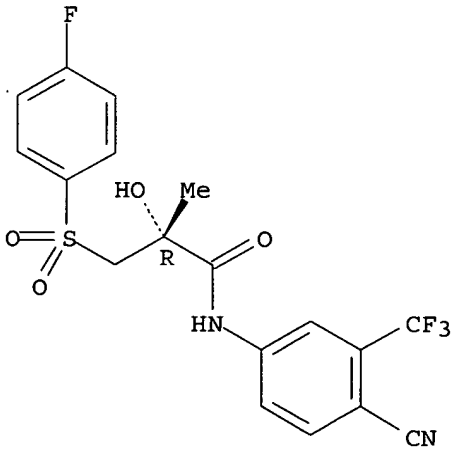
IT **90357-06-5P**, Bicalutamide **113299-40-4P**, (R)-Bicalutamide
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of bicalutamide by coupling of N-[4-cyano-3-(trifluoromethyl)phenyl]-2-methyl-2-orixanecarboxamide or -3-(halo or mesyloxy)-2-hydroxy-2-methylpropanamide with sodium p-fluorobenzenesulfinate)

RN 90357-06-5 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



RN 113299-40-4 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L28 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:300625 HCAPLUS
DOCUMENT NUMBER: 138:321017
TITLE: Process for making bicalutamide using a p-fluorobenzenesulfinic acid salt.
INVENTOR(S): Thijs, Lambertus; Keltjens, Rolf; Ettema, Gerrit Jan Bouke
PATENT ASSIGNEE(S): Synthon B.V., Neth.
SOURCE: U.S. Pat. Appl. Publ., 24 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003073742	A1	20030417	US 2002-261492	20021002
US 6818766	B2	20041116		
WO 2004031136	A1	20040415	WO 2003-EP11166	20031001
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1546093	A1	20050629	EP 2003-757932	20031001
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004068135	A1	20040408	US 2003-682530	20031010

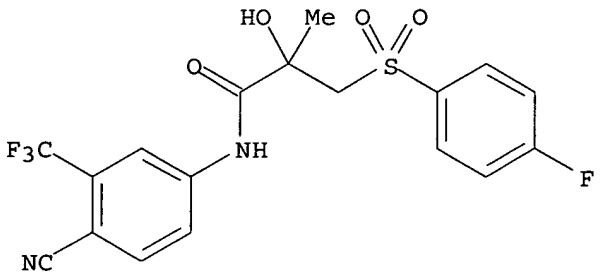
PRIORITY APPLN. INFO.: US 2002-261492 A 20021002
WO 2003-EP11166 W 20031001

OTHER SOURCE(S): CASREACT 138:321017; MARPAT 138:321017

AB Title process is claimed. Thus, N-[4-cyano-3-(trifluoromethyl)phenyl]-2-methyl-2-oxiranecarboxamide (preparation given), Na p-fluorobenzenesulfinate, and Bu4NBr were refluxed together for 96 h to give 48% bicalutamide.

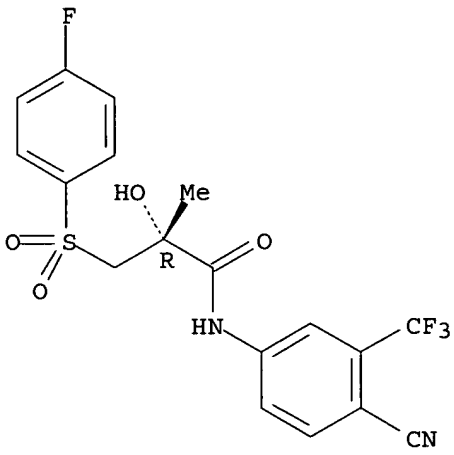
IT **90357-06-5P**, Bicalutamide **113299-40-4P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for making bicalutamide using a p-fluorobenzenesulfinic acid salt)

RN 90357-06-5 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)

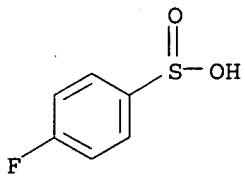


RN 113299-40-4 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (2R)- (9CI) (CA INDEX NAME)

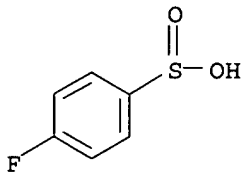
Absolute stereochemistry. Rotation (-).



IT **369-51-7D**, p-Fluorobenzenesulfinic acid, salts **824-80-6**, Sodium p-fluorobenzenesulfinate
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for making bicalutamide using a p-fluorobenzenesulfinic acid salt)
RN 369-51-7 HCAPLUS
CN Benzenesulfinic acid, 4-fluoro- (9CI) (CA INDEX NAME)



RN 824-80-6 HCAPLUS
CN Benzenesulfinic acid, 4-fluoro-, sodium salt (9CI) (CA INDEX NAME)

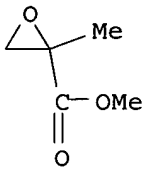


● Na

IT **58653-97-7P 512776-89-5P 512776-90-8P**

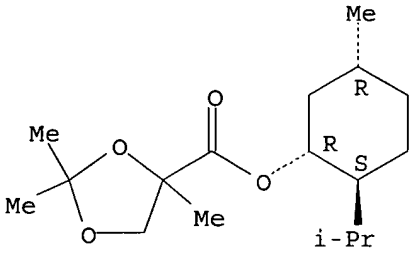
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for making bicalutamide using a p-fluorobenzenesulfinic acid salt)

RN 58653-97-7 HCAPLUS
CN Oxiranecarboxylic acid, 2-methyl-, methyl ester (9CI) (CA INDEX NAME)

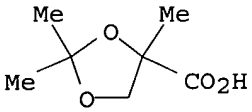


RN 512776-89-5 HCAPLUS
CN 1,3-Dioxolane-4-carboxylic acid, 2,2,4-trimethyl-, (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 512776-90-8 HCAPLUS
CN 1,3-Dioxolane-4-carboxylic acid, 2,2,4-trimethyl-, sodium salt (9CI) (CA INDEX NAME)



● Na

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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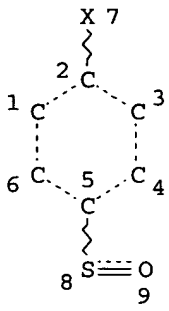
L2 STR



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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
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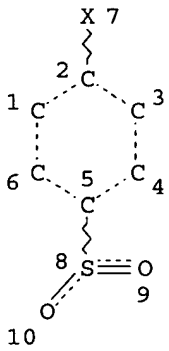

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DEFAULT ECLEVEL IS LIMITED

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STEREO ATTRIBUTES: NONE
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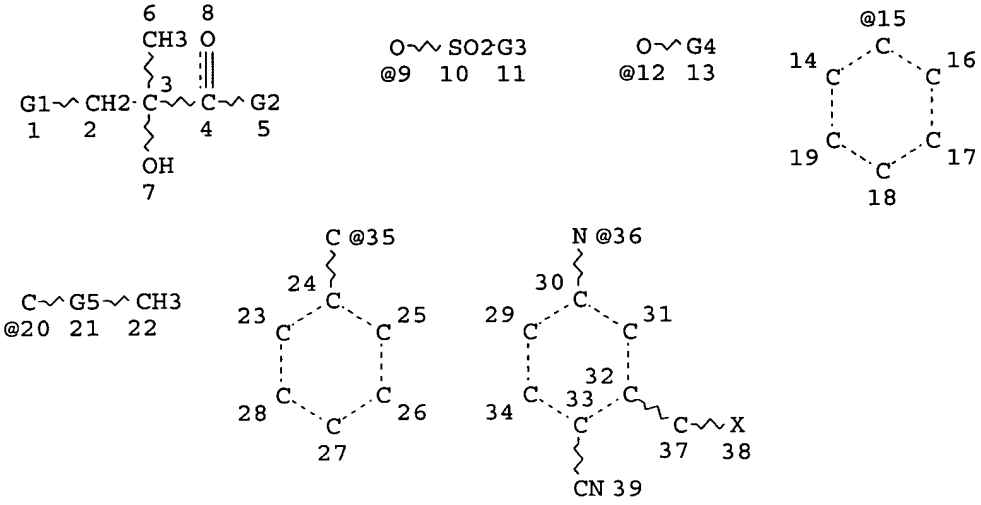
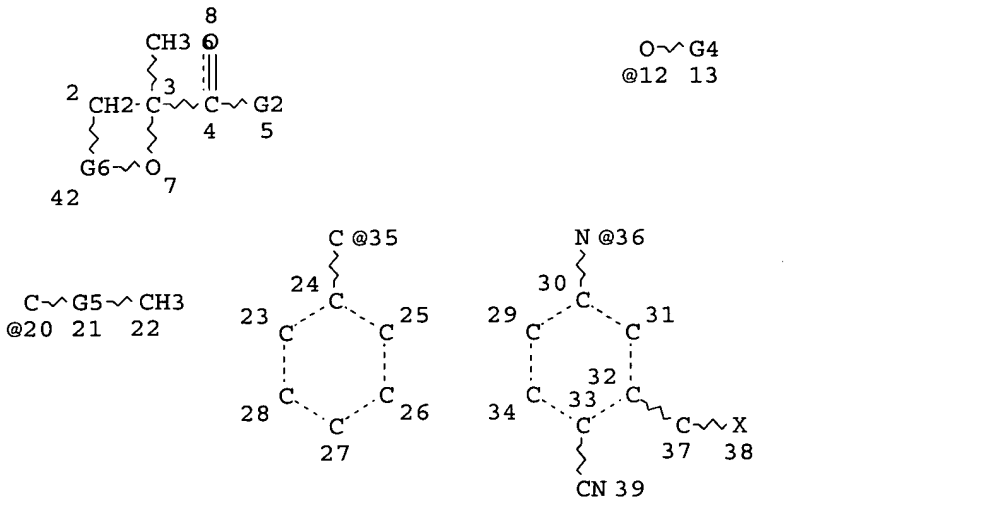


VAR G1=X/9
VAR G2=OH/12
VAR G3=OH/ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/15
VAR G4=ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/20/CB/35/36
REP G5=(3-4) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 39

STEREO ATTRIBUTES: NONE
L10 STR

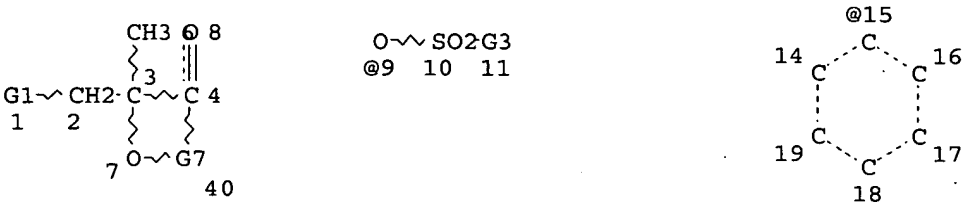


VAR G2=OH/12
VAR G4=ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/20/CB/35/36
REP G5=(3-4) C
REP G6=(0-3) A

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE
L11 STR



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VAR G3=OH/ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/15
REP G7=(2-7) A
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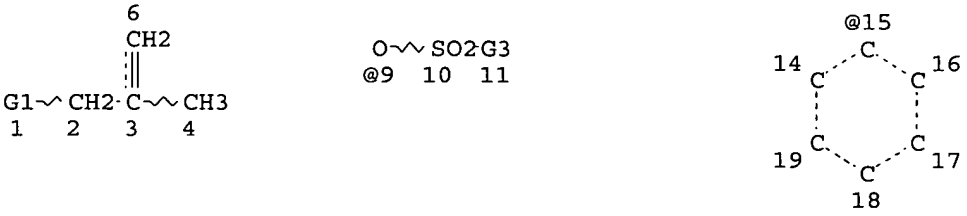
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L12 STR



VAR G1=X/9
VAR G3=OH/ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/15
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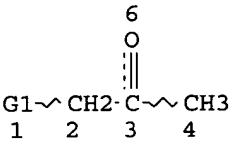
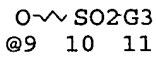
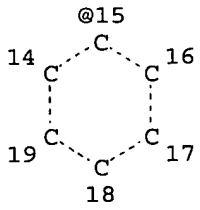
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L13 STR



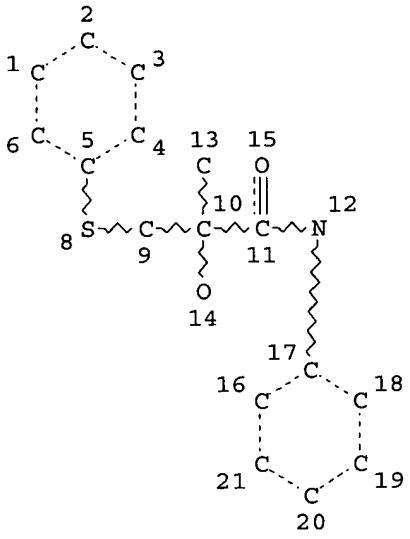




VAR G1=X/9
VAR G3=OH/ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/15
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L17 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
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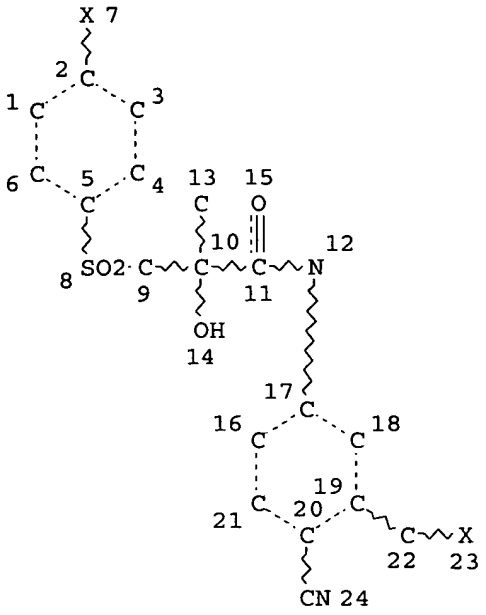
L22 210 SEA FILE=REGISTRY SSS FUL L17
L23 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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L26	15691	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L5
L27	8894	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L20
L36	27	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L24/P
L37	14	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L25 AND L26
L38	12	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L25 AND L27
L40	39	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L36 OR L37 OR L38

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=>

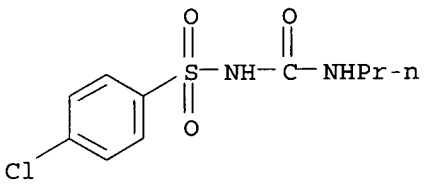
=> d his l41

(FILE 'HCAPLUS' ENTERED AT 09:26:06 ON 20 AUG 2005)
L41 14 S L40 AND PD=<OCTOBER 9, 2002

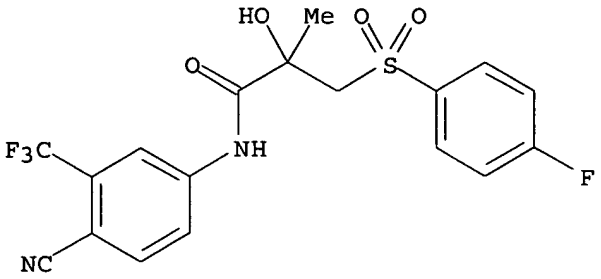
=> d ibib abs hitstr l41 1-14

L41 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:895868 HCAPLUS
DOCUMENT NUMBER: 139:143316
TITLE: ADME evaluation 2. A computer model for the prediction of intestinal absorption in humans
AUTHOR(S): Klopman, Gilles; Stefan, Liliana R.; Saiakhov, Roustem

D.
CORPORATE SOURCE: Department of Chemistry, Case Western Reserve University, Cleveland, OH, 44106, USA
SOURCE: European Journal of Pharmaceutical Sciences (**2002**), 17(4-5), 253-263
CODEN: EPSCED; ISSN: 0928-0987
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Purpose: To develop a computational method to rapidly evaluate human intestinal absorption, one of the drug properties included in the term ADME (Absorption, Distribution, Metabolism, Excretion). Poor ADME properties are the most important reason for drug failure in clin. development. Methods: The model developed is based on a modified contribution group method in which the basic parameters are structural descriptors identified by the case program, together with the number of hydrogen bond donors. Results: The human intestinal absorption model is a quant. structure-activity relationship (QSAR) that includes 37 structural descriptors derived from the chemical structures of a data set containing 417 drugs. The model was able to predict the percentage of drug absorbed from the gastrointestinal tract with an r2 of 0.79 and a standard deviation of 12.32% of the compds. from the training set. The standard deviation for an external test set (50 drugs) was 12.34%. Conclusions: The availability of reliable and fast models like the one we propose here to predict ADME/Tox properties could help speed up the process of finding compds. with improved properties, ultimately making the entire drug discovery process shorter and more cost efficient.
IT **94-20-2**, Chlorpropamide **90357-06-5**, Bicalutamide
RL: PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(computer model for prediction of intestinal absorption in humans)
RN 94-20-2 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-[(propylamino)carbonyl]- (9CI) (CA INDEX NAME)

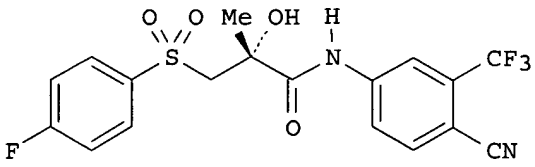


RN 90357-06-5 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)

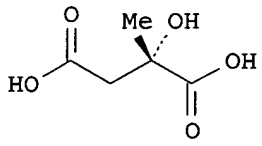


REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:509907 HCAPLUS
DOCUMENT NUMBER: 137:384623
TITLE: Syntheses of enantiomerically pure (R)- and (S)-bicalutamide
AUTHOR(S): James, Kenneth D.; Ekwuribe, Nnochiri N.
CORPORATE SOURCE: Department of Innovation, Nobex Corporation, Durham, NC, 27713, USA
SOURCE: Tetrahedron (**2002**), 58(29), 5905-5908
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:384623
GI



I



II

AB The racemic antiandrogen bicalutamide is the leading antiandrogen used for the treatment of prostate cancer. The (R)-isomer possesses virtually all of the activity, but both isomers are metabolized by the liver. A convenient synthetic route to the active enantiomer would be an attractive option for patients who are hepatically impaired. We now demonstrate a rather short synthesis of (R)-bicalutamide (I), starting with naturally occurring (S)-citramalic acid (II). The authors have also used this procedure to synthesized the less active (S)-bicalutamide from the

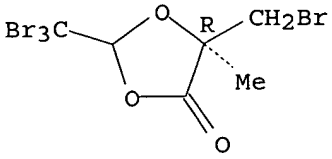
unnatural (R)-citramalic acid.

IT **335595-50-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(syntheses of enantiomerically pure (R)- and (S)-bicalutamide)

RN 335595-50-1 HCAPLUS

CN 1,3-Dioxolan-4-one, 5-(bromomethyl)-5-methyl-2-(tribromomethyl)-, (5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

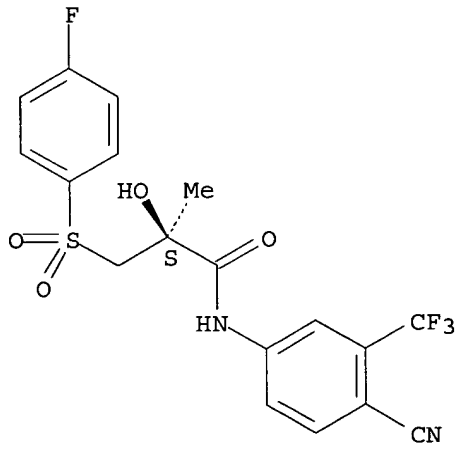


IT **113299-38-0P 113299-40-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(syntheses of enantiomerically pure (R)- and (S)-bicalutamide)

RN 113299-38-0 HCAPLUS

CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (2S)- (9CI) (CA INDEX NAME)

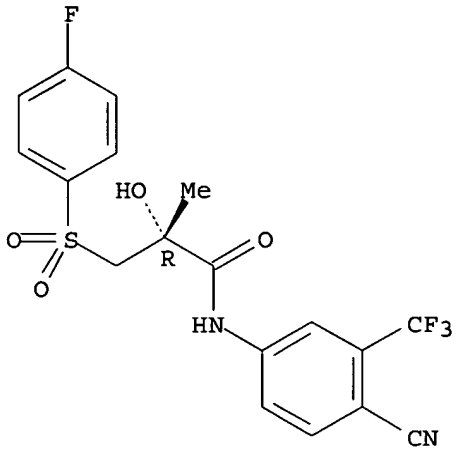
Absolute stereochemistry. Rotation (+).



RN 113299-40-4 HCAPLUS

CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



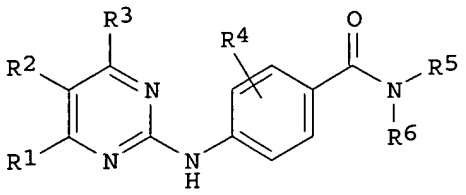
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:449662 HCAPLUS
DOCUMENT NUMBER: 137:33310
TITLE: Preparation of anilinopyrimidines as IKK inhibitors
INVENTOR(S): Kois, Adam; MacFarlane, Karen J.; Satoh, Yoshitaka; Bhagwat, Shripad S.; Parnes, Jason S.; Palanki, Moorthy S. S.; Erdman, Paul E.
PATENT ASSIGNEE(S): Signal Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 194 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002046171	A2	20020613	WO 2001-US46403		20011205 <--
WO 2002046171	A3	20030123			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
US 2003203926	A1	20031030	US 2001-4642		20011204
CA 2431160	AA	20020613	CA 2001-2431160		20011205 <--
AU 2002020195	A5	20020618	AU 2002-20195		20011205 <--
EP 1349841	A2	20031008	EP 2001-999564		20011205
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004523497	T2	20040805	JP 2002-547910		20011205
PRIORITY APPLN. INFO.:			US 2000-251816P	P	20001206
			WO 2001-US46403	W	20011205

OTHER SOURCE(S): MARPAT 137:33310

GI



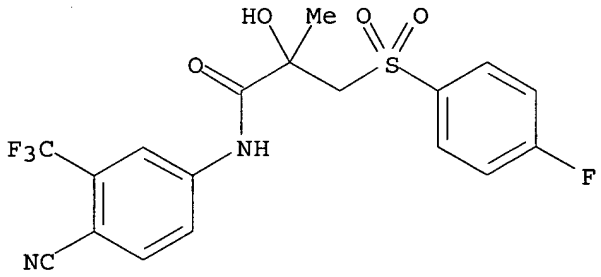
I

AB The title compds. [I; R1 = (un)substituted (hetero)aryl; R2 = H; R3 = H, alkyl; R4 = halo, OH, alkyl, alkoxy; R5, R6 = R8, (CH2)aCOR9, (CH2)aCO2R9, etc.; or NR5R6 = (un)substituted heterocycle; R8, R9 = H, alkyl, aryl, etc.; a = 0-4] having activity as inhibitors of IKK, particularly IKK-2, were prepared E.g., a multi-step synthesis of I [R1 = 4-ClC6H4; R2-R6 = H] having an IC50 of ≤ 1 μM in the IKK-2 enzyme assay, was given. Such compds. I have utility in the treatment of a wide range of conditions that are responsive to IKK inhibition. Thus, methods of treating such conditions are also disclosed, as are pharmaceutical compns. containing one or more compds. of the above compds.

IT **90357-06-5**, Bicalutamide
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anticancer agent; preparation of anilinopyrimidines as IKK inhibitors)

RN 90357-06-5 HCAPLUS

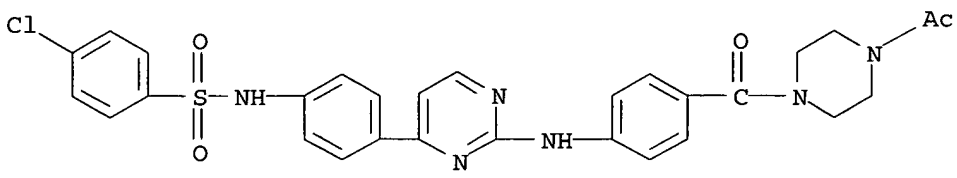
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



IT **434948-10-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of anilinopyrimidines as IKK inhibitors)

RN 434948-10-4 HCAPLUS

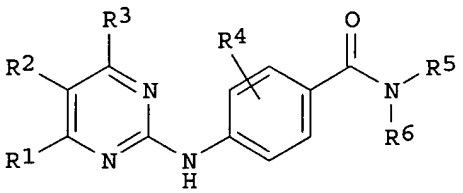
CN Piperazine, 1-acetyl-4-[4-[[4-[4-[[(4-chlorophenyl)sulfonyl]amino]phenyl]-2-pyrimidinyl]amino]benzoyl]- (9CI) (CA INDEX NAME)



L41 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:449661 HCAPLUS
DOCUMENT NUMBER: 137:33309
TITLE: Preparation of anilinopyrimidines as JNK pathway inhibitors
INVENTOR(S): Kois, Adam; MacFarlane, Karen J.; Satoh, Yoshitaka; Bhagwat, Shripad S.; Parnes, Jason S.; Palanki, Moorthy S. S.; Erdman, Paul E.
PATENT ASSIGNEE(S): Signal Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 199 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002046170	A2	20020613	WO 2001-US46402		20011205 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2430966	AA	20020613	CA 2001-2430966		20011205 <--
AU 2002027214	A5	20020618	AU 2002-27214		20011205 <--
EP 1349840	A2	20031008	EP 2001-996103		20011205
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004534728	T2	20041118	JP 2002-547909		20011205
PRIORITY APPLN. INFO.:			US 2000-251904P	P	20001206
			WO 2001-US46402	W	20011205

OTHER SOURCE(S): MARPAT 137:33309
GI



I

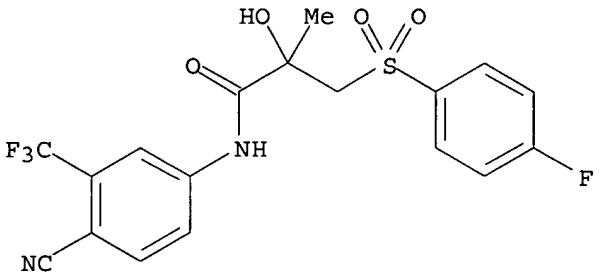
AB The title compds. [I; R1 = (un)substituted (hetero)aryl; R2 = H; R3 = H, alkyl; R4 = halo, OH, alkyl, alkoxy; R5, R6 = R8, (CH2)aCOR9, (CH2)aCO2R9, etc.; or NR5R6 = (un)substituted heterocycle; R8, R9 = H, alkyl, aryl, etc.; a = 0-4] having activity as inhibitors of the JNK pathway, were prepared E.g., a multi-step synthesis of I [R1 = 4-ClC6H4; R2-R6 = H] having an IC50 of ≤ 10 μM in the JNK2 assay, was given. Such compds. I have utility in the treatment of a wide range of conditions that are responsive to inhibition of the JNK pathway. Thus, methods of

treating such conditions are also disclosed, as are pharmaceutical compns. containing one or more compds. of the above compds.

IT **90357-06-5**, Bicalutamide
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anticancer agent; preparation of anilinopyrimidines as JNK pathway inhibitors)

RN 90357-06-5 HCAPLUS

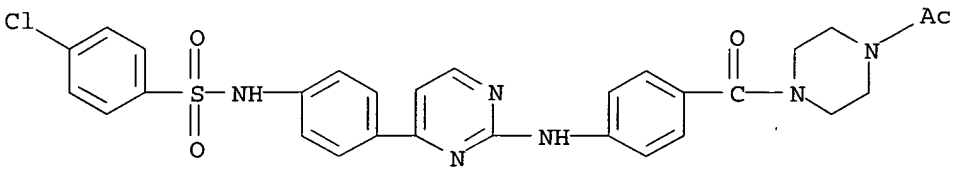
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



IT **434948-10-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of anilinopyrimidines as JNK pathway inhibitors)

RN 434948-10-4 HCAPLUS

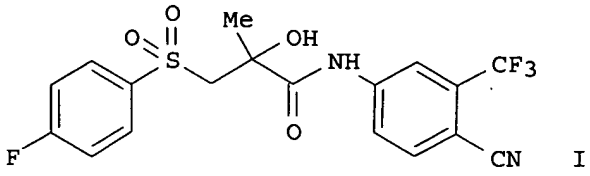
CN Piperazine, 1-acetyl-4-[4-[[4-[4-[[(4-chlorophenyl)sulfonyl]amino]phenyl]-2-pyrimidinyl]amino]benzoyl]- (9CI) (CA INDEX NAME)



L41 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	2002:414656 HCAPLUS
DOCUMENT NUMBER:	137:262824
TITLE:	A two-step synthesis of the anti-cancer drug (R,S)-bicalutamide
AUTHOR(S):	James, Kenneth D.; Ekwuribe, Nnochiri N.
CORPORATE SOURCE:	Department of Innovation, Nobex Corporation, Durham, NC, 27713, USA
SOURCE:	Synthesis (**2002**), (7), 850-852 CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER:	Georg Thieme Verlag
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 137:262824

GI



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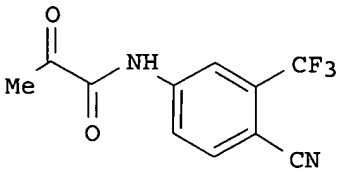


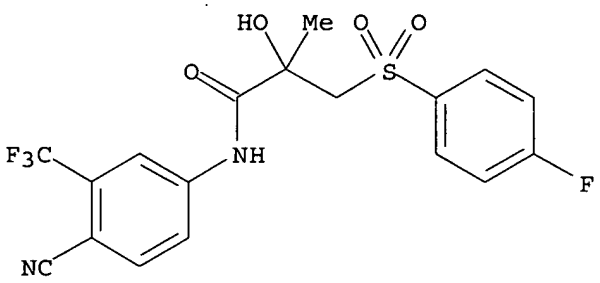
II

AB A short, efficient synthesis of the non-steroidal antiandrogen (R,S)-bicalutamide I is presented. This new route generates bicalutamide in only two steps with an overall yield of 73%. The key step is a 1,2-addition of 4-fluorophenyl methylsulfone to a keto-amide II.

IT **90357-06-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(two-step synthesis of the anti-cancer drug (R,S)-bicalutamide via addition reaction of 4-fluorophenyl methylsulfone to keto-amide)

RN 90357-06-5 HCAPLUS

CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:240719 HCAPLUS

DOCUMENT NUMBER: 136:262992

TITLE: Process for the preparation of N-(substituted phenyl)-3-alkyl-, aryl- and heteroarylsulfonyl-2-hydroxy-2-alkyl- and haloalkylpropanamide antiandrogenic compounds

INVENTOR(S): Chen, Bang-Chi; Sundeen, Joseph E.; Zhao, Rulin

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2

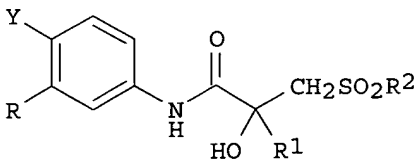
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002024638	A1	20020328	WO 2001-US42171		20010917 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2423158	AA	20020328	CA 2001-2423158		20010917 <--
US 2002086902	A1	20020704	US 2001-953759		20010917 <--
US 6562994	B2	20030513			
EP 1322603	A1	20030702	EP 2001-975752		20010917
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004509164	T2	20040325	JP 2002-529051		20010917
CN 1501912	A	20040602	CN 2001-818933		20010917
BR 2001014277	A	20041221	BR 2001-14277		20010917
PRIORITY APPLN. INFO.:			US 2000-234121P	P	20000921
			WO 2001-US42171	W	20010917

OTHER SOURCE(S): CASREACT 136:262992; MARPAT 136:262992
GI



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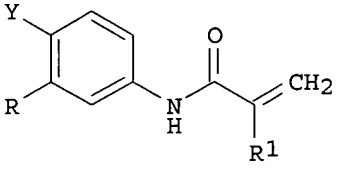
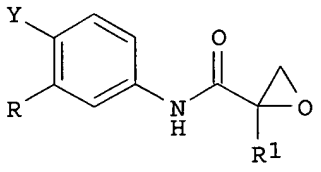
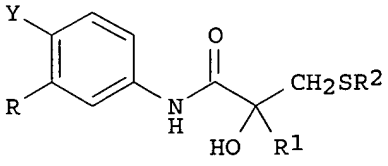


II



III



IV

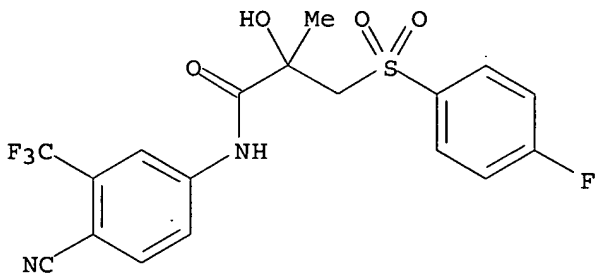
AB The title compds. [I; Y = cyano, nitro, perfluoroalkyl, alkylcarbonyl, alkoxycarbonyl, alkylsulfonyl; R = perfluoroalkyl, cyano, nitro, alkylcarbonyl, alkoxycarbonyl, alkyl, alkoxy; R1 = (halo)alkyl; R2 = alkyl, aryl, heteroaryl; e.g., bicalutamide], useful for the treatment of androgen-mediated diseases (no data), are prepared without the use of chromatog. sepns. and expensive starting materials by phenylating propenamides H2NCOC(R1):CH2 (e.g., methacrylamide) with leaving group-substituted benzenes 1,2,4-C6H3Y(R)X (X = F, Cl, Br, I, SO3R3; R3 =

alkyl, aryl; e.g., 4-fluoro-2-trifluoromethylbenzonitrile) so as to form a N-phenyl-substituted propenamides [II; e.g., N-[4-Cyano-3-(trifluoromethyl)phenyl]methacrylamide] which are then oxidized into the corresponding epoxides [III; e.g., N-[4-Cyano-3-(trifluoromethyl)phenyl]methacrylamide epoxide], converted into thioethers [IV; e.g., N-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)thio]-2-hydroxy-2-methylpropanamide] by reaction with mercaptans R2SH (e.g., 4-fluorothiophenol), and then oxidized into their corresponding sulfones.

IT **90357-06-5P**, Bicalutamide
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of N-(substituted phenyl)-3-alkyl-, aryl- and heteroarylsulfonyl-2-hydroxy-2-alkyl- and haloalkylpropanamide antiandrogenic compds.)

RN 90357-06-5 HCAPLUS

CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:359958 HCAPLUS
DOCUMENT NUMBER: 134:366692
TITLE: Resolution of intermediates in the synthesis of enantiomeric bicalutamide and analogs
INVENTOR(S): Ekwuribe, Nnochiri N.; James, Kenneth D.
PATENT ASSIGNEE(S): Nobex Corporation, USA
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001034563	A1	20010517	WO 2000-US41609	20001025 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2389100	AA	20010517	CA 2000-2389100	20001025 <--

BR 2000015124	A	20020702	BR 2000-15124		20001025 <--
EP 1224167	A1	20020724	EP 2000-989719		20001025 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL					
JP 2003513955	T2	20030415	JP 2001-536512		20001025
US 6593492	B1	20030715	US 2000-695884		20001025
NZ 518552	A	20031031	NZ 2000-518552		20001025
ZA 2002003228	A	20030723	ZA 2002-3228		20020423
NO 2002001999	A	20020620	NO 2002-1999		20020426 <--
PRIORITY APPLN. INFO.:			US 1999-161884P	P	19991027
			WO 2000-US41609	W	20001025

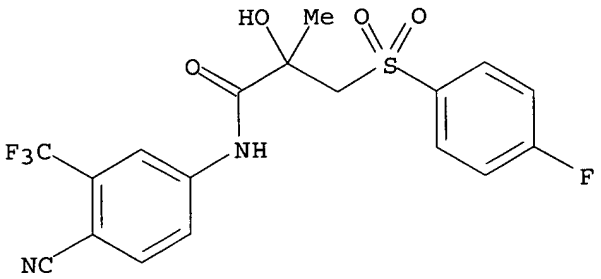
OTHER SOURCE(S): MARPAT 134:366692

AB Title enantiomeric acylanilides were prepared by resolution of R4ZZ1Z2CR1(OH)CO2H [R1 = (halo)alkyl; R4 = (hydroxy)alkyl, alkenyl, (un)substituted Ph, etc.; Z = bond or alkylene; Z1 = O, SO0-2, (alkyl)imino; Z2 = alkylene] followed by amidation.

IT **90357-06-5P**, Bicalutamide
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(resolution of intermediates in the synthesis of enantiomeric bicalutamide and analogs)

RN 90357-06-5 HCAPLUS

CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

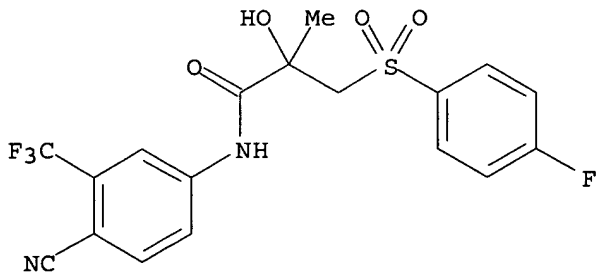
ACCESSION NUMBER:	2001:306242 HCAPLUS
DOCUMENT NUMBER:	135:87257
TITLE:	Homology Modeling Using Multiple Molecular Dynamics Simulations and Docking Studies of the Human Androgen Receptor Ligand Binding Domain Bound to Testosterone and Nonsteroidal Ligands
AUTHOR(S):	Marhefka, Craig A.; Moore, Bob M. ,II; Bishop, Thomas C.; Kirkovsky, Leonid; Mukherjee, Arnab; Dalton, James T.; Miller, Duane D.
CORPORATE SOURCE:	Department of Pharmaceutical Sciences College of Pharmacy, University of Tennessee-Health Science Center, Memphis, TN, 38163, USA
SOURCE:	Journal of Medicinal Chemistry (**2001**), 44(11), 1729-1740 CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER:	American Chemical Society
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB To facilitate the rational design of novel and more potent androgen receptor ligands, three-dimensional models for the human androgen receptor ligand binding domain bound to testosterone have been developed. These models of the androgen receptor were based on the crystal structure of the highly homologous human progesterone receptor ligand binding domain. The homol. modeled androgen receptor was refined using unrestrained multiple mol. dynamics simulations in explicit solvent. Key H-bonding partners with the 17-hydroxy group and 3-keto group of testosterone are Asn705 and Thr877, and Gln711 and Arg752, resp. These models show the presence of a unique unoccupied cavity within the androgen receptor binding pocket which may be valuable in the development of novel selective androgen receptor ligands. A qual. anal. of amino acid mutations within the hAR binding pocket that affect ligand binding are consistent with these androgen receptor models. In addition to testosterone, the binding modes of several hydroxyflutamide-like nonsteroidal ligands for the androgen receptor are investigated using flexible docking with FlexX followed by refinement of the initial complexes with mol. dynamics simulations. These docking studies indicate that Asn705 is an important determinant in binding hydroxyflutamide and its derivs. by participating in H-bond interactions with the α-hydroxy moiety of these ligands. In addition, the nitro functionality mimics the 3-keto group of the natural ligand testosterone and is involved in H-bonding interactions with Gln711 and Arg752. From these docking studies, we suggest a mechanism for the enantioselective binding of chiral hydroxyflutamide derivs. and expand upon the previously reported structure-activity relationship for hydroxyflutamide and its derivs.

IT **90357-06-5**, Bicalutamide
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(homol. modeling using multiple mol. dynamics simulations and docking studies of human androgen receptor ligand binding domain bound to testosterone and hydroxyflutamide derivative ligands)

RN 90357-06-5 HCAPLUS

CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)

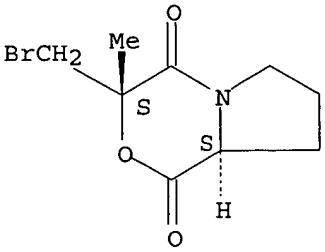


IT **106089-19-4 106138-80-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(in hydroxyflutamide derivative preparation for human androgen receptor ligand-binding structure-activity mol. dynamics simulation and docking studies)

RN 106089-19-4 HCAPLUS

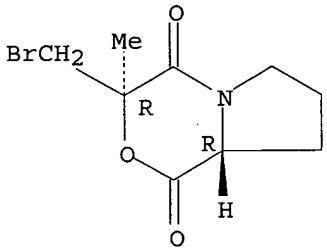
CN 1H-Pyrrolo[2,1-c][1,4]oxazine-1,4(3H)-dione, 3-(bromomethyl)tetrahydro-3-methyl-, (3S,8aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



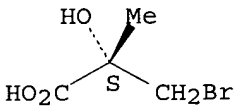
RN 106138-80-1 HCAPLUS
CN 1H-Pyrrolo[2,1-c][1,4]oxazine-1,4(3H)-dione, 3-(bromomethyl)tetrahydro-3-methyl-, (3R,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



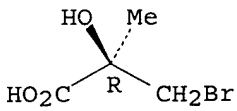
IT **106089-20-7P 261904-39-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in hydroxyflutamide derivative preparation for human androgen receptor ligand-binding structure-activity mol. dynamics simulation and docking studies)
RN 106089-20-7 HCAPLUS
CN Propanoic acid, 3-bromo-2-hydroxy-2-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 261904-39-6 HCAPLUS
CN Propanoic acid, 3-bromo-2-hydroxy-2-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

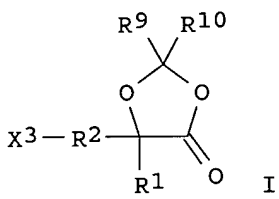
L41 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:300671 HCAPLUS
DOCUMENT NUMBER: 134:326279
TITLE: Asymmetric synthesis and antiandrogenic use of enantiomers of Casodex (bicalutamide) and derivatives from enantiomers of citramalic acid or proline.
INVENTOR(S): Ekwuribe, Nnochiri
PATENT ASSIGNEE(S): Nobex Corporation, USA
SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

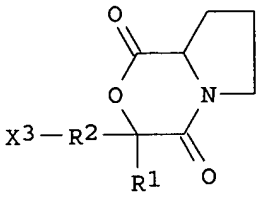
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
WO 2001028990	A2	20010426	WO 2000-US41233	20001018	<--
WO 2001028990	A3	20010907			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2387570	AA	20010426	CA 2000-2387570	20001018	<--
EP 1222165	A2	20020717	EP 2000-982690	20001018	<--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL					
BR 2000014889	A	20021231	BR 2000-14889	20001018	
JP 2003512351	T2	20030402	JP 2001-531790	20001018	
US 6583306	B1	20030624	US 2000-691621	20001018	
NZ 518392	A	20040227	NZ 2000-518392	20001018	
ZA 2002002947	A	20030715	ZA 2002-2947	20020415	
NO 2002001831	A	20020619	NO 2002-1831	20020418	<--
US 2004030130	A1	20040212	US 2003-444343	20030523	

PRIORITY APPLN. INFO.:	US 1999-160412P	P	19991019
	US 2000-691621	A3	20001018
	WO 2000-US41233	W	20001018

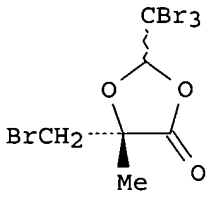
OTHER SOURCE(S): CASREACT 134:326279; MARPAT 134:326279
GI



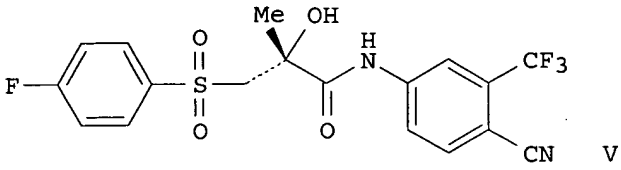
I



II



IV



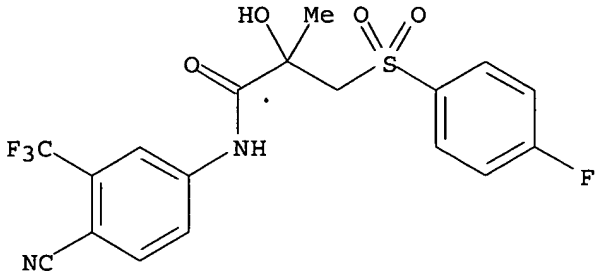
V

AB A method of synthesizing pure enantiomers of acylanilides such as Casodex (bicalutamide) is disclosed. The method involves contacting certain ring compds. including I, II, or similar gem-disubstituted epoxides with nucleophiles R7-R6-X1H under conditions sufficient to provide a compound R7-R6-X2-R2-C(OH)(R1)-CO2H [wherein; R1 is alkyl or haloalkyl up to C4; R2 is alkyl up to C6; R6 is a bond or alkyl up to C6; R7 is alk(en)yl, hydroxyalkyl, etc. or R7 is Ph (substituted with up to 3 substituents chosen from H, halo, nitro, carboxy, carbamoyl, etc.); X1 is O, SO0-2, or (alkyl)imino; X2 is O, S(O)0-2 or (oxidized)(alkyl)imino; X3 is a leaving group]. The starting ring compds. are those that, when opened, provide a substituent -R2-C(OH)(R1)-R3 [wherein; R3 is CH2OR4, where R4 is H, PhCH2, C(O)CH3, C(O)OR5, where R5 is H or alkyl]. In an exemplary embodiment, readily available (S)-citramalic acid is reacted with bromal to yield I (R9 = H, R10 is CBr3, R1 is β-Me, R2 is α-CH2 and X3 is CO2H; III). Compound III is condensed with 2-mercaptopyridine-N-oxide using DCC in CBrCl3 (solvent) at reflux which resulted in α-bromination/decarboxylation to IV. Intermediate IV was sequentially treated with base and 4-fluorobenzenethiol, coupled with 4-amino-2-trifluoromethylbenzonitrile and oxidized with mCPBA to give (R)-Casodex (V). The order of steps in the conversion of I or II to compds. exemplified by V may vary (e.g. substitution and oxidation of a sidechain of I may precede ring opening). The conversion of (R)-citramalic acid to (S)-Casodex is also claimed. Addnl., the invention mentions a modification of a route previously described for the transformation of (R)- and (S)-proline to (R)- and (S)-Casodex that improves yield proceeding through a proline-derived intermediate II. Biol. data comparing (R)-, (S)- and (±)-Casodex, synthesized by this method, in lowering testosterone response showed (R)-Casodex to be substantially more potent than the (S)-isomer.

IT **90357-06-5**, Casodex
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(asym. synthesis (and use) of (R)- and (S)-Casodex (bicalutamide) from (S)- and (R)-citramalic acid)

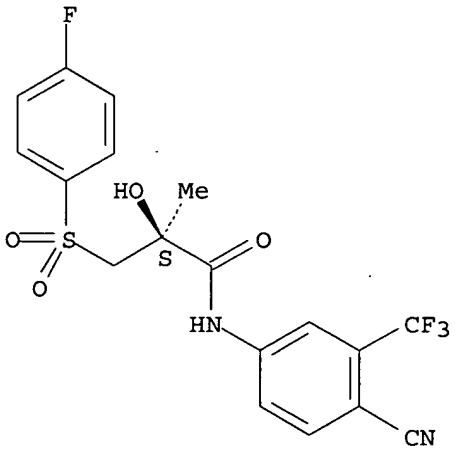
RN 90357-06-5 HCAPLUS

CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



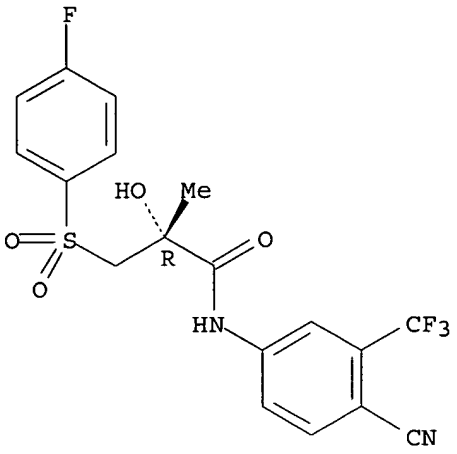
IT **113299-38-0P**, S-Casodex **113299-40-4P**, R-Casodex
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(asym. synthesis (and use) of (R)- and (S)-Casodex (bicalutamide) from (S)- and (R)-citramalic acid)
RN 113299-38-0 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



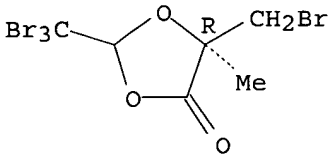
RN 113299-40-4 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **335595-50-1P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis (and use) of (R)- and (S)-Casodex (bicalutamide) from (S)- and (R)-citramalic acid)
RN 335595-50-1 HCAPLUS
CN 1,3-Dioxolan-4-one, 5-(bromomethyl)-5-methyl-2-(tribromomethyl)-, (5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L41 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:12441 HCAPLUS
DOCUMENT NUMBER: 134:86040
TITLE: Preparation of bicalutamide enantiomers
INVENTOR(S): Soros, Bela; Tuba, Zoltan; Galik, Gyorgy; Bor, Adam; Demeter, Adam; Trischler, Ferenc; Horvath, Janos; Brlik, Janos
PATENT ASSIGNEE(S): Richter Gedeon Vegyeszeti Gyar Rt., Hung.
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000608	A1	20010104	WO 2000-HU49	20000526 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,

LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA,
ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

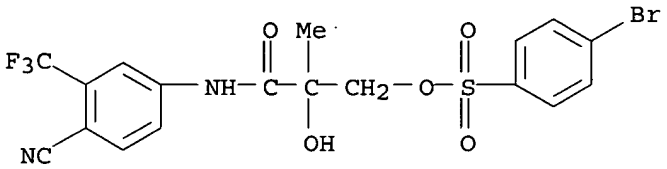
EP 1189898	A1	20020327	EP 2000-937111	20000526	<--
EP 1189898	B1	20030312			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
AT 234294	E	20030315	AT 2000-937111	20000526	
ES 2188550	T3	20030701	ES 2000-937111	20000526	
PRIORITY APPLN. INFO.:			HU 1999-1937	A 19990610	
			WO 2000-HU49	W 20000526	

OTHER SOURCE(S): CASREACT 134:86040

AB Racemic HOCH2CMe(OH)CO2H was optically resolved and the enantiomers treated with SOCL2 to give the dioxothiolanonecarbonyl chloride which was amidated by H2NC6H3(CF3)(CN)-3,4. The deprotected dihydroxyamide was O-acylated by RSO2Cl (R = 4-Me- or -BrC6H4) and the product thioetherified by 4-FC6H4SNa to give, after oxidation, the title compds.

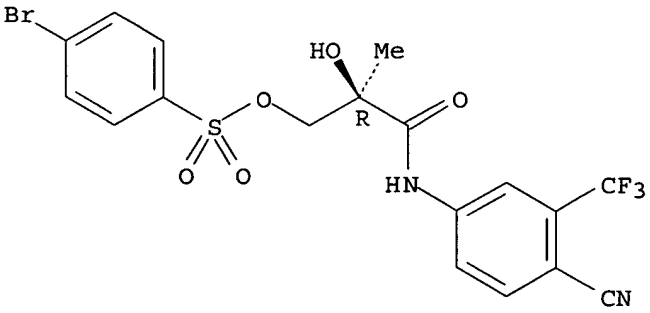
IT **316374-01-3P 316374-02-4P 316374-03-5P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bicalutamide enantiomers)

RN 316374-01-3 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 3-[[4-cyano-3-(trifluoromethyl)phenyl]amino]-2-hydroxy-2-methyl-3-oxopropyl ester (9CI) (CA INDEX NAME)



RN 316374-02-4 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, (2R)-3-[[4-cyano-3-(trifluoromethyl)phenyl]amino]-2-hydroxy-2-methyl-3-oxopropyl ester (9CI) (CA INDEX NAME)

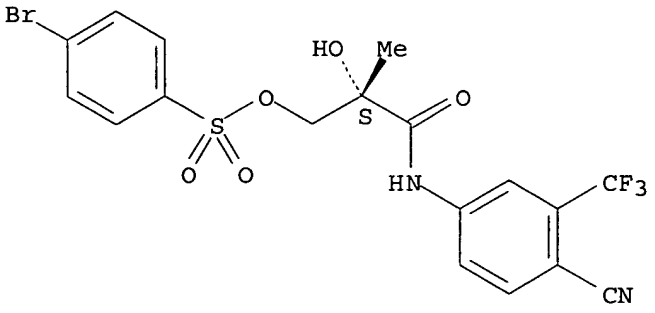
Absolute stereochemistry. Rotation (-).



RN 316374-03-5 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, (2S)-3-[[4-cyano-3-

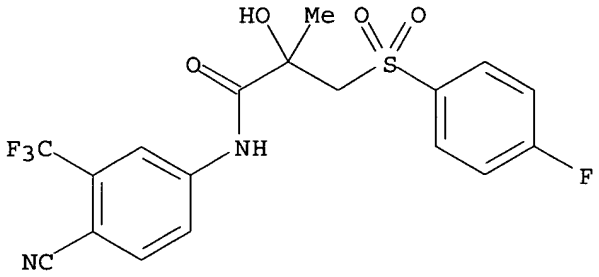
(trifluoromethyl)phenyl]amino]-2-hydroxy-2-methyl-3-oxopropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



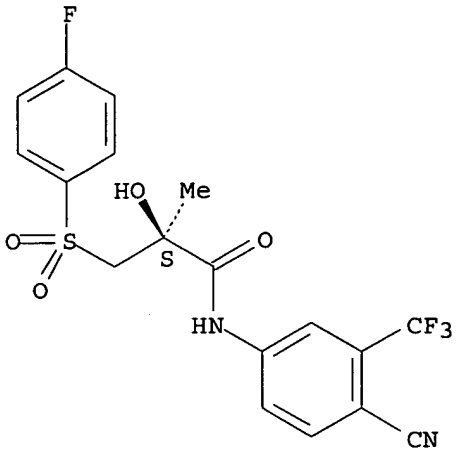
IT **90357-06-5P 113299-38-0P 113299-40-4P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of bicalutamide enantiomers)

RN 90357-06-5 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



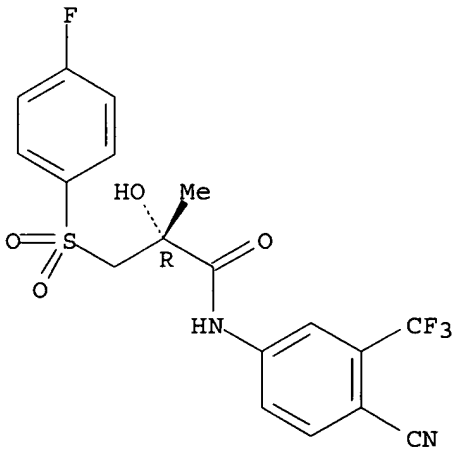
RN 113299-38-0 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 113299-40-4 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:804210 HCAPLUS
DOCUMENT NUMBER: 130:49289
TITLE: Nonsteroidal radiolabeled androgen receptor agonist/antagonist compounds, preparation, and use in prostate cancer imaging
INVENTOR(S): Miller, Duane D.; Kirkovsky, Leonid I.; Dalton, James T.; Mukherjee, Arnab
PATENT ASSIGNEE(S): The University of Tennessee Research Corp., USA
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9855153	A1	19981210	WO 1998-US11483	19980604 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9877231	A1	19981221	AU 1998-77231	19980604 <--
US 6019957	A	20000201	US 1998-90425	19980604 <--
US 2002098148	A1	20020725	US 1999-461543	19991215 <--
PRIORITY APPLN. INFO.:			US 1997-49376P	P 19970604
			US 1998-90425	A3 19980604
			WO 1998-US11483	W 19980604

OTHER SOURCE(S): MARPAT 130:49289

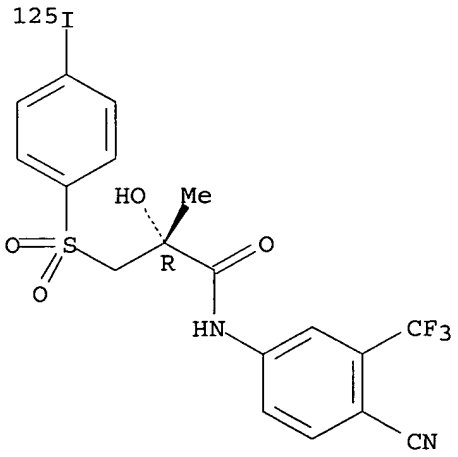
AB Anilide radiolabeled androgen receptor ligands are provided, as is their use in methods of imaging the prostate. Compound preparation is also described.

IT **217170-51-9P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(nonsteroidal radiolabeled androgen receptor agonist/antagonist compds., preparation, and use in prostate cancer imaging)

RN 217170-51-9 HCAPLUS

CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-2-hydroxy-3-[[4-(iodo-125I)phenyl]sulfonyl]-2-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:161557 HCAPLUS

DOCUMENT NUMBER: 108:161557

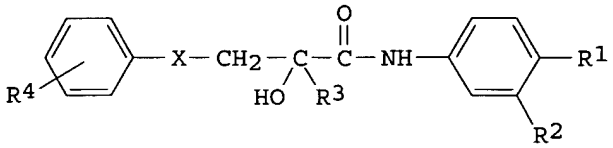
TITLE: Nonsteroidal antiandrogens. Synthesis and structure-activity relationships of 3-substituted

derivatives of 2-hydroxypropionanilides

AUTHOR(S): Tucker, Howard; Crook, J. W.; Chesterson, G. J.
CORPORATE SOURCE: Pharm. Div., Imp. Chem. Ind. PLC, Macclesfield/Cheshire, AK10 4TG, UK

SOURCE: Journal of Medicinal Chemistry (1988), 31(5), 954-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:161557

GI



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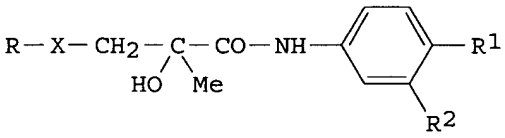
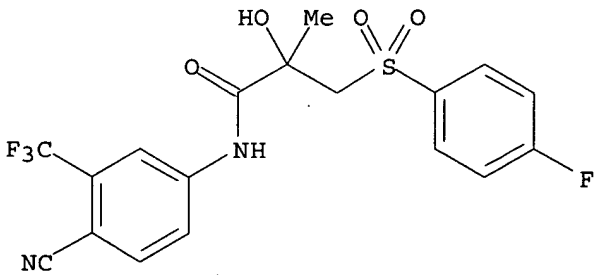


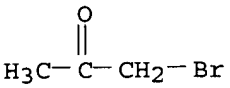
II

AB A series of hydroxypropionanilides of general structure I and II (R1,R2 = NO2, CF3, CN, or Cl; R3 = CF3 or CH3; R4 = H, Cl, F, NO2, CN, MeO, or MeS; X = S, SO, or SO2; and R = alkyl or heterocyclic derivs.) were prepared and tested for antiandrogen activity by their effects on accessory sex organs in rats. A series of compds. where R3 = CF3 generally exhibited partial androgen agonist activity, whereas those compds. where R3 = CH3 were pure antagonists. Optimization of the latter series of compds. led to novel, potent antiandrogens which were peripherally selective.

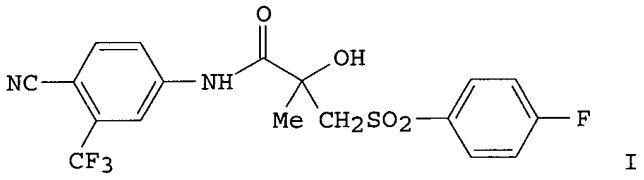
IT **90357-06-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antiandrogen activity of, structure in relation to)
RN 90357-06-5 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



IT **598-31-2**, Bromoacetone
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thiols)
RN 598-31-2 HCAPLUS
CN 2-Propanone, 1-bromo- (8CI, 9CI) (CA INDEX NAME)



L41 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:150026 HCAPLUS
DOCUMENT NUMBER: 108:150026
TITLE: Resolution of the non-steroidal antiandrogen 4'-cyano-3-(4-fluorophenylsulfonyl)-2-hydroxy-2-methyl-3'-(trifluoromethyl)propionanilide and the determination of the absolute configuration of the active enantiomer
AUTHOR(S): Tucker, Howard; Chesterson, Glynne J.
CORPORATE SOURCE: Pharm. Div., Imp. Chem. Ind. PLC, Mereside/Macclesfield/Cheshire, SK10 4TG, UK
SOURCE: Journal of Medicinal Chemistry (**1988**), 31(4), 885-7
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:150026
GI

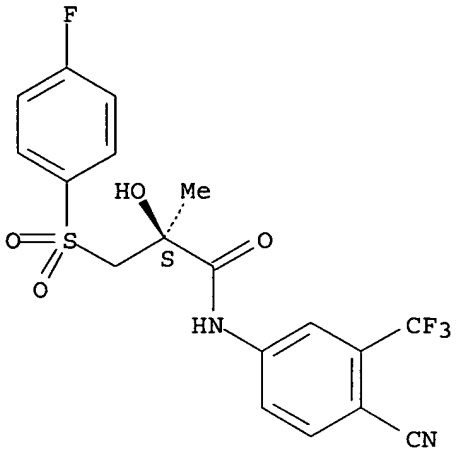


I

AB The nonsteroidal antiandrogen 4'-cyano-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-3'-(trifluoromethyl)propionanilide (I) has been resolved by chromatog. separation of the diastereomeric (R)-camphanyl esters of the precursor thioether followed by hydrolysis and oxidation of the isolated enantiomers. In addition, an asym. synthesis of (S)-3-bromo-2-hydroxy-2-methylpropanoic acid and subsequent conversion into the (S)-sulfone has established that the more potent enantiomer of I has the R absolute configuration.

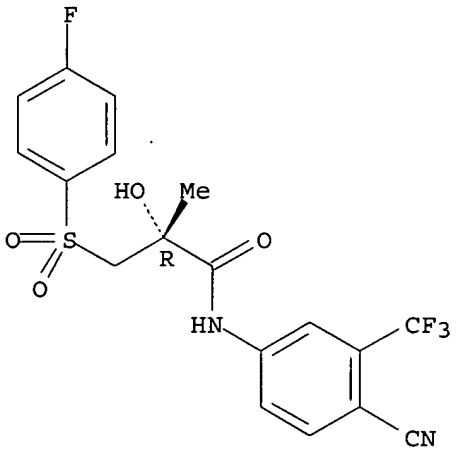
IT **113299-38-0P 113299-40-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antiandrogen activity of)
RN 113299-38-0 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



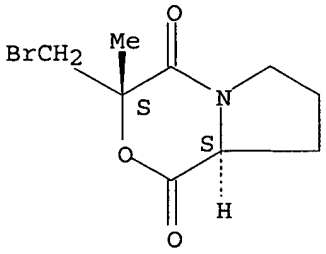
RN 113299-40-4 HCAPLUS
CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



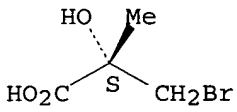
IT **106089-19-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 106089-19-4 HCAPLUS
CN 1H-Pyrrolo[2,1-c][1,4]oxazine-1,4(3H)-dione, 3-(bromomethyl)tetrahydro-3-methyl-, (3S,8aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **106089-20-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, chlorination, and amidation of)
RN 106089-20-7 HCAPLUS
CN Propanoic acid, 3-bromo-2-hydroxy-2-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

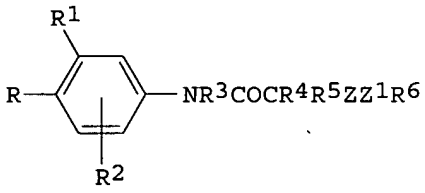


L41 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:454739 HCAPLUS
DOCUMENT NUMBER: 101:54739
TITLE: Amide derivatives
INVENTOR(S): Tucker, Howard
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK
SOURCE: Eur. Pat. Appl., 53 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 100172	A1	19840208	EP 1983-303998	19830708 <--
EP 100172	B1	19870812		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 28864	E	19870815	AT 1983-303998	19830708 <--
IL 69217	A1	19870331	IL 1983-69217	19830713 <--
ZA 8305182	A	19840530	ZA 1983-5182	19830715 <--
US 4636505	A	19870113	US 1983-514332	19830715 <--
NO 8302599	A	19840124	NO 1983-2599	19830718 <--
NO 164974	B	19900827		
NO 164974	C	19901205		
AU 8316937	A1	19840126	AU 1983-16937	19830718 <--
AU 556328	B2	19861030		
HU 32058	O	19840628	HU 1983-2531	19830718 <--
HU 191296	B	19870227		
FI 8302644	A	19840124	FI 1983-2644	19830720 <--
FI 83770	B	19910515		
FI 83770	C	19910826		

JP 59033250	A2	19840223	JP 1983-131085		19830720 <--
JP 04032061	B4	19920528			
CA 1249823	A1	19890207	CA 1983-432811		19830720 <--
ES 524392	A1	19851101	ES 1983-524392		19830722 <--
ES 539614	A1	19860601	ES 1985-539614		19850116 <--
ES 539615	A1	19860601	ES 1985-539615		19850116 <--
ES 544189	A1	19860916	ES 1985-544189		19850614 <--
JP 02131462	A2	19900521	JP 1989-230574		19890907 <--
PRIORITY APPLN. INFO.:			GB 1982-21421	A	19820723
			EP 1983-303998	A	19830708

GI



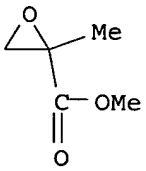
I

AB Antiandrogenic (no data) alkananilides including I [R = alkanoyl, halo, cyano, NO2, alkylthio, alkylsulfinyl, alkylsulfonyl, PhS, PhSO, PhSO2, etc.; R1 = H, alkyl, alkoxy, R; R2 = H, halo; R3 = H, alkyl; R4 = H, OH, alkoxy, acyloxy; R5 = alkyl, haloalkyl; R4R5 = CO2; R6 = (un)substituted alkyl, alkenyl, Ph, naphthyl, heterocyclyl; Z = bond, alkylene; Z1 = O, S, S(O), SO2, NR7; R7 = H, alkyl] (124 compds.) were prepared Thus, Me 2,3-epoxy-2-methylpropionate, prepared by epoxidn. of H2C:CMeCO2Me, was treated with NaH and PhSH to give PhSCH2CMe(OH)CO2Me. This was saponified to give the free acid which was treated with SOCl2 and 4,3-(NC)(F3C)C6H3NH2 to give 4,3-(NC)(F3C)C6H3NHCOCMe(OH)CH2SPh.

IT **58653-97-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and condensation of, with thiols)

RN 58653-97-7 HCAPLUS

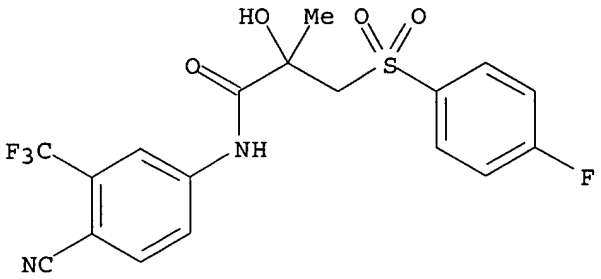
CN Oxiranecarboxylic acid, 2-methyl-, methyl ester (9CI) (CA INDEX NAME)



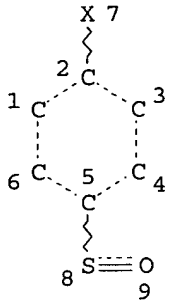
IT **90357-06-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 90357-06-5 HCAPLUS

CN Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



=> => d stat que
L2 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
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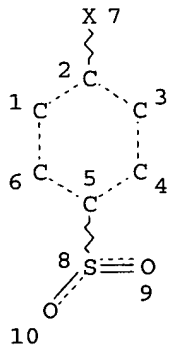
L4 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
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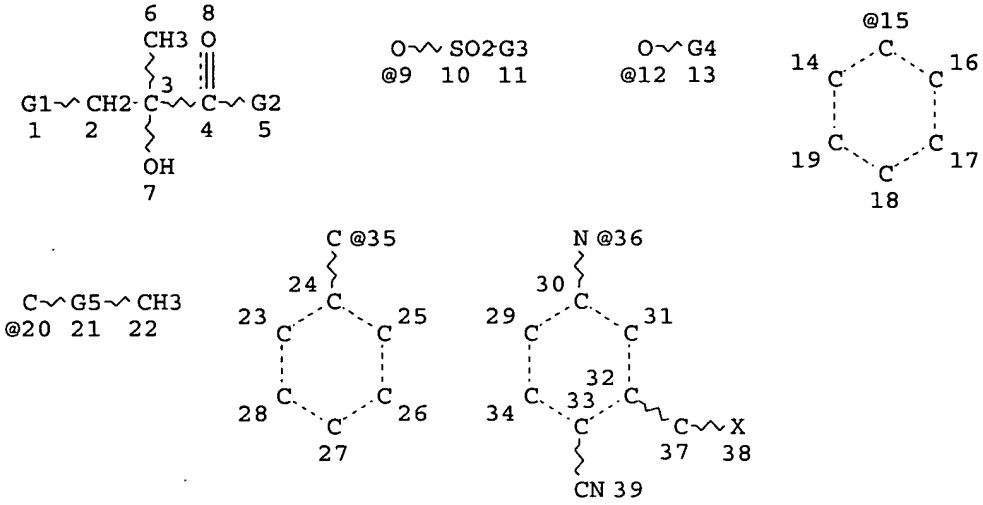
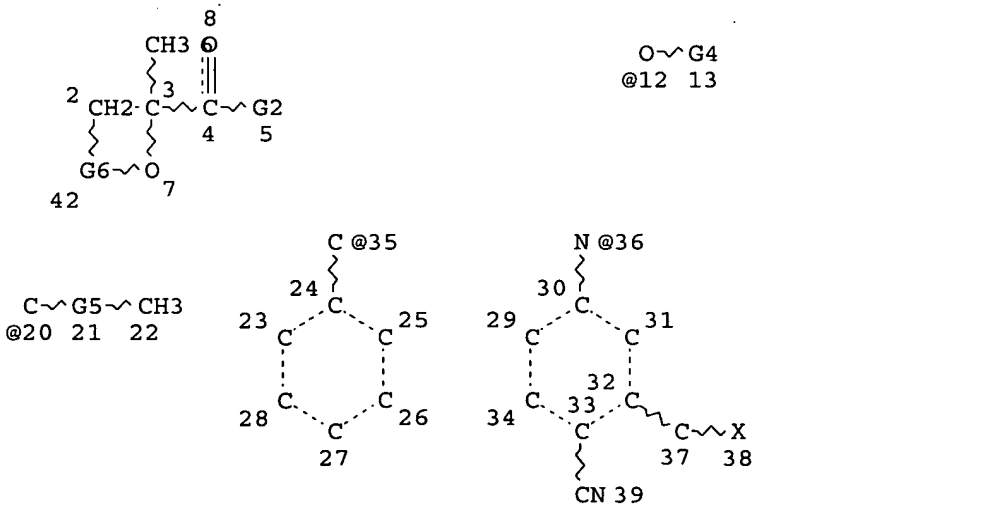
L9 STR



VAR G1=X/9
VAR G2=OH/12
VAR G3=OH/ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/15
VAR G4=ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/20/CB/35/36
REP G5=(3-4) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 39

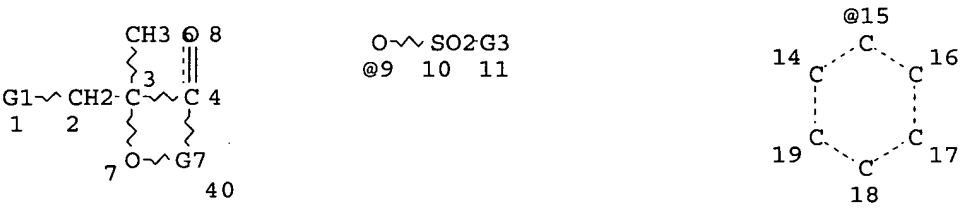
STEREO ATTRIBUTES: NONE
L10 STR



VAR G2=OH/12
VAR G4=ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/20/CB/35/36
REP G5=(3-4) C
REP G6=(0-3) A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

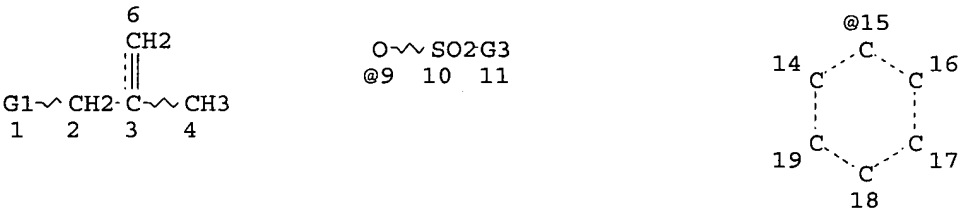
STEREO ATTRIBUTES: NONE
L11 STR



VAR G1=X/9
VAR G3=OH/ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/15
REP G7=(2-7) A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

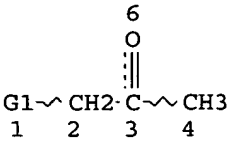
STEREO ATTRIBUTES: NONE
L12 STR

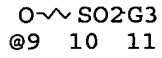


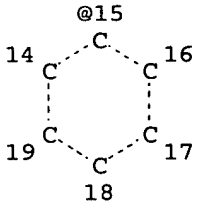
VAR G1=X/9
VAR G3=OH/ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/15
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L13 STR



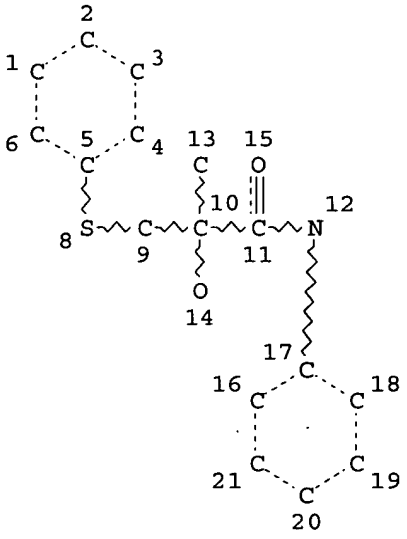




VAR G1=X/9
VAR G3=OH/ME/ET/I-PR/N-PR/I-BU/N-BU/T-BU/S-BU/15
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L17 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
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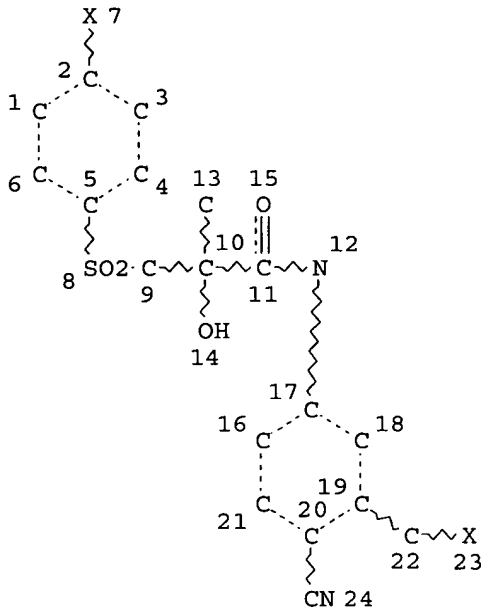
L22 210 SEA FILE=REGISTRY SSS FUL L17
L23 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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L25	484	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L24
L26	15691	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L5
L27	8894	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L20
L28	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L25 AND L26 AND L27
L32	89	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L26 AND L27
L36	27	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L24/P
L37	14	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L25 AND L26
L38	12	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L25 AND L27
L39	70	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L32 AND PD=<OCTOBER 9, 2002
L40	39	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L36 OR L37 OR L38
L41	14	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L40 AND PD=<OCTOBER 9, 2002
L42	70	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L39 NOT (L41 OR L28)
L45	3967	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L26(L)REACTANT/RL
L46	6032	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L27(L)REACTANT/RL
L47	32	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON (L45 AND L46) AND L42

=> d ibib abs hitstr l47 1-32

L47 ANSWER 1 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:796768 HCAPLUS
DOCUMENT NUMBER: 138:338037
TITLE: Herbicidal thiochroman and dihydrobenzothiophene-N,N-disubstituted pyrazolinones
AUTHOR(S): Anon.

CORPORATE SOURCE: UK
SOURCE: Research Disclosure (**2002**), 461(Sept.), P1676-P1692 (No. 461084)
CODEN: RSDSBB; ISSN: 0374-4353
PUBLISHER: Kenneth Mason Publications Ltd.
DOCUMENT TYPE: Journal; Patent
LANGUAGE: English
PATENT INFORMATION:

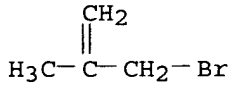
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RD 461084		20020910		
PRIORITY APPLN. INFO.:			RD 2002-461084	20020910

OTHER SOURCE(S): CASREACT 138:338037

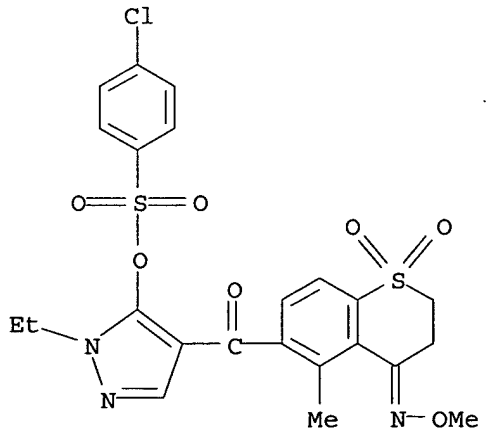
AB Numerous N,N-disubstituted pyrazolinone compds., which were highly effective in controlling undesirable plant species, are disclosed. The methods for the control of undesirable plant species which could also be useful in the presence of an essential agronomic crop are presented.

IT **1458-98-6**, 3-Bromo-2-methyl-1-propene **516500-85-9**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepns. of thiochroman and dihydrobenzothiophene-N,N-disubstituted pyrazolinone derivs. as herbicidal agents)

RN 1458-98-6 HCAPLUS
CN 1-Propene, 3-bromo-2-methyl- (9CI) (CA INDEX NAME)



RN 516500-85-9 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 4-[[3,4-dihydro-4-(methoxyimino)-5-methyl-1,1-dioxido-2H-1-benzothiopyran-6-yl]carbonyl]-1-ethyl-1H-pyrazol-5-yl ester (9CI) (CA INDEX NAME)

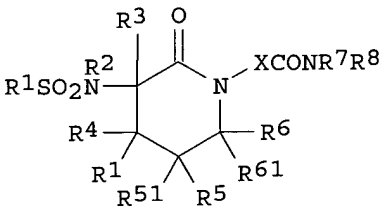


L47 ANSWER 2 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:594840 HCAPLUS
DOCUMENT NUMBER: 137:154858
TITLE: Preparation of arylsulfonamidopiperidones as inhibitors of Factor Xa.

INVENTOR(S): Stein, Philip P.; O'Connor, Stephen P.; Lawrence, R. Michael; Shi, Yan
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 246 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002060894	A2	20020808	WO 2002-US2542		20020128 <--
WO 2002060894	A3	20021219			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2436774	AA	20020808	CA 2002-2436774		20020128 <--
EP 1358178	A2	20031105	EP 2002-717381		20020128
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004518688	T2	20040624	JP 2002-561043		20020128
US 6555542	B1	20030429	US 2002-59621		20020129
PRIORITY APPLN. INFO.:			US 2001-264964P	P	20010130
			WO 2002-US2542	W	20020128

OTHER SOURCE(S): MARPAT 137:154858
GI



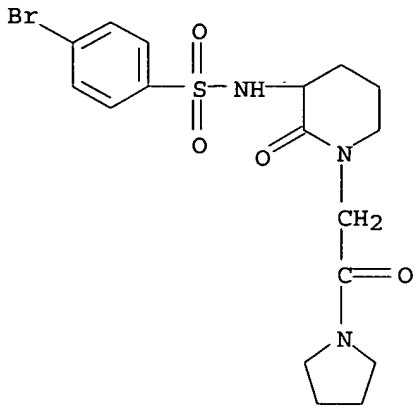
I

AB Title compds. [I; X = (substituted) (CH2)m; m = 1-3; R1 = (substituted) alkyl, alkenyl, alkynyl, aryl, heteroaryl, etc.; R2, R3 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R4, R41, R5, R51 = H, OH, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, alkoxy, etc.; R6, R61 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R7, R8 = (substituted) (CH2)nH; n = 1-4; R7R8N = (substituted) cycloheteroalkyl], were prepared as cardiovascular agents (no data). 974 I, including (II), were prepared

IT **445271-15-8P 445274-86-2P 445277-69-0P 445278-08-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

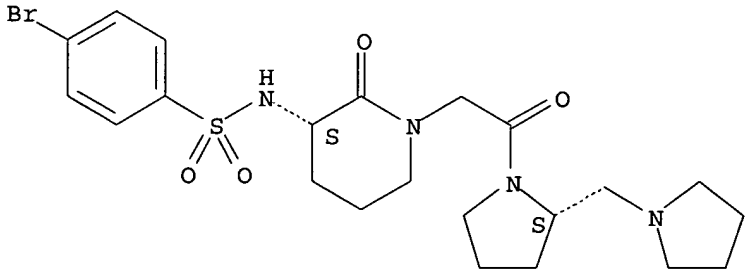
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arylsulfonamidopiperidones as inhibitors of Factor Xa)

RN 445271-15-8 HCAPLUS
CN Pyrrolidine, 1-[[3-[[(4-bromophenyl)sulfonyl]amino]-2-oxo-1-piperidinyl]acetyl]- (9CI) (CA INDEX NAME)



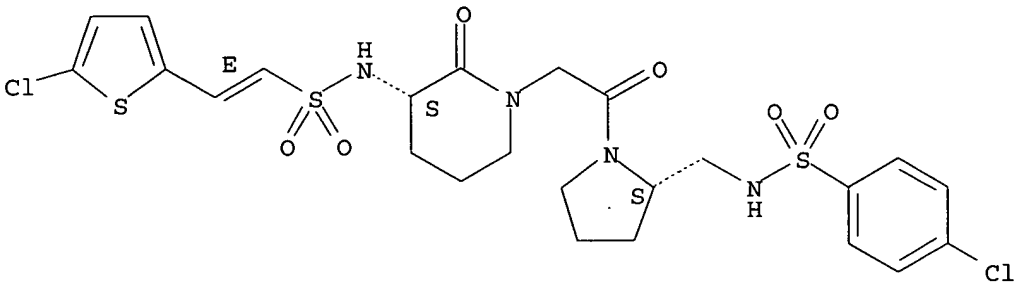
RN 445274-86-2 HCAPLUS
CN Pyrrolidine, 1-[[(3S)-3-[[(4-bromophenyl)sulfonyl]amino]-2-oxo-1-piperidinyl]acetyl]-2-(1-pyrrolidinylmethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



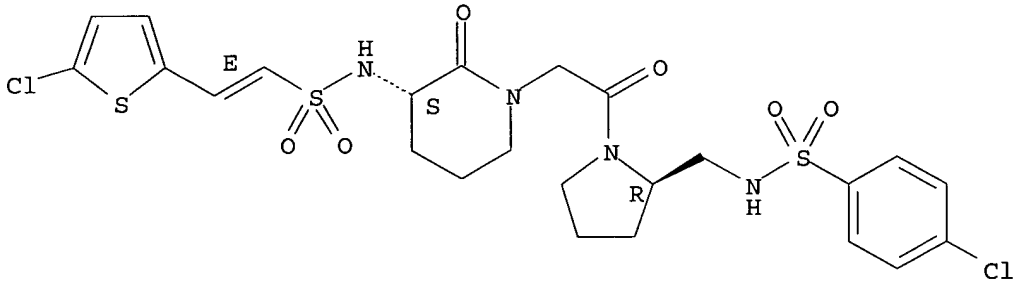
RN 445277-69-0 HCAPLUS
CN 2-Pyrrolidinemethanamine, N-[(4-chlorophenyl)sulfonyl]-1-[[(3S)-3-[[[(1E)-2-(5-chloro-2-thienyl)ethenyl]sulfonyl]amino]-2-oxo-1-piperidinyl]acetyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

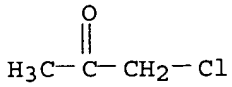


RN 445278-08-0 HCAPLUS
CN 2-Pyrrolidinemethanamine, N-[(4-chlorophenyl)sulfonyl]-1-[[(3S)-3-[[[(1E)-2-(5-chloro-2-thienyl)ethenyl]sulfonyl]amino]-2-oxo-1-piperidinyl]acetyl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

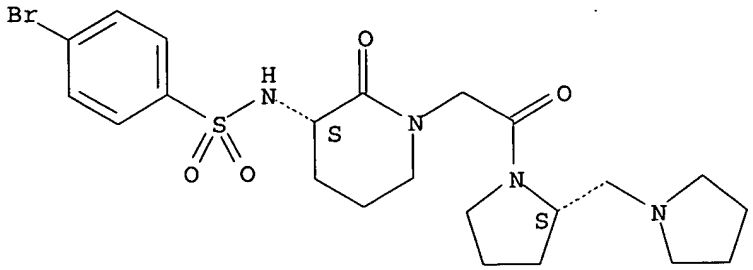


IT **78-95-5**, Chloroacetone **445274-86-2D**, resin-bound
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation of arylsulfonamidopiperidones as inhibitors of Factor Xa)
RN 78-95-5 HCAPLUS
CN 2-Propanone, 1-chloro- (8CI, 9CI) (CA INDEX NAME)



RN 445274-86-2 HCAPLUS
CN Pyrrolidine, 1-[[(3S)-3-[[(4-bromophenyl)sulfonyl]amino]-2-oxo-1-piperidinyl]acetyl]-2-(1-pyrrolidinylmethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L47 ANSWER 3 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:575041 HCAPLUS
DOCUMENT NUMBER: 137:140338
TITLE: Preparation of aminoethanol derivatives as cholesteryl ester transfer protein inhibitors for treatment of hyperlipidemia, etc.
INVENTOR(S): Kori, Masakuni; Hamamura, Kazumasa; Fuse, Hiromitsu; Yamamoto, Toshihiro
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 748 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002059077	A1	20020801	WO 2002-JP532	20020125 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2002293764	A2	20021009	JP 2002-17487	20020125 <--
EP 1362846	A1	20031119	EP 2002-710345	20020125
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004127574	A1	20040701	US 2003-470351	20030725
PRIORITY APPLN. INFO.:			JP 2001-19280 A	20010126
			WO 2002-JP532 W	20020125

OTHER SOURCE(S): MARPAT 137:140338

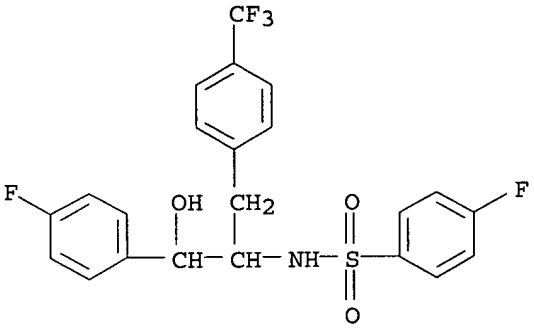
AB The title compds. Ar1CH(OR'')CH(CH2Ar2)NR'R [Ar1 represents an optionally substituted aromatic ring group; Ar2 represents a substituted aromatic ring group; OR'' represents optionally protected hydroxy; R represents acyl; and R' represents hydrogen or optionally substituted hydrocarbyl] are prepared Compds. of this invention in vitro showed IC50 values of 0.0084 μM to 0.4 μM against cholesteryl ester transfer protein. A process for preparing the title compds. is claimed.

IT **444912-33-8P**
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);

PREP (Preparation); USES (Uses)
(preparation of aminoethanol derivs. as cholesteryl ester transfer protein inhibitors for treatment of hyperlipidemia)

RN 444912-33-8 HCAPLUS

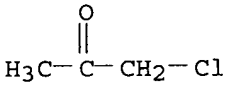
CN Benzenesulfonamide, 4-fluoro-N-[2-(4-fluorophenyl)-2-hydroxy-1-[[4-(trifluoromethyl)phenyl]methyl]ethyl]- (9CI) (CA INDEX NAME)



IT **78-95-5**, Chloroacetone
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation of aminoethanol derivs. as cholesteryl ester transfer protein inhibitors for treatment of hyperlipidemia)

RN 78-95-5 HCAPLUS

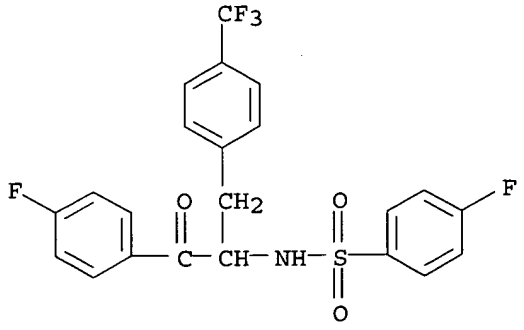
CN 2-Propanone, 1-chloro- (8CI, 9CI) (CA INDEX NAME)



IT **444913-21-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aminoethanol derivs. as cholesteryl ester transfer protein inhibitors for treatment of hyperlipidemia)

RN 444913-21-7 HCAPLUS

CN Benzenesulfonamide, 4-fluoro-N-[2-(4-fluorophenyl)-2-oxo-1-[[4-(trifluoromethyl)phenyl]methyl]ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 4 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:772163 HCAPLUS
DOCUMENT NUMBER: 135:318510
TITLE: Preparation of arylpyridazinones as prostaglandin endoperoxide H synthase biosynthesis inhibitors
INVENTOR(S): Black, Lawrence A.; Basha, Anwer; Kolasa, Teodozyj; Kort, Michael E.; Liu, Huaqing; McCarty, Catherine M.; Patel, Meena; Rohde, Jeffrey J.; Coghlan, Michael J.; Stewart, Andrew O.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: U.S., 129 pp., Cont.-in-part of U.S. Ser. No. 261,872, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

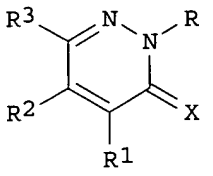
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6307047	B1	20011023	US 1999-427768	19991027 <--
TR 200000478	T2	20020422	TR 2000-200000478	19980810 <--
CA 2347982	AA	20000504	CA 1999-2347982	19991027 <--
WO 2000024719	A1	20000504	WO 1999-US25234	19991027 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9965230	A1	20000515	AU 1999-65230	19991027 <--
AU 773237	B2	20040520		
EP 1124804	A1	20010822	EP 1999-953259	19991027 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9914858	A	20020205	BR 1999-14858	19991027 <--
TR 200101765	T2	20020221	TR 2001-200101765	19991027 <--
JP 2003512292	T2	20030402	JP 2000-578289	19991027
ZA 2001003310	A	20020723	ZA 2001-3310	20010423 <--
NO 2001002061	A	20010627	NO 2001-2061	20010426 <--
BG 105523	A	20011231	BG 2001-105523	20010519 <--
US 2002013318	A1	20020131	US 2001-871195	20010531 <--
US 2002028938	A1	20020307	US 2001-870838	20010531 <--
US 2003225276	A1	20031204	US 2003-417959	20030417
US 2004158064	A1	20040812	US 2003-464928	20030619

PRIORITY APPLN. INFO.:		
US 1997-56733P	P	19970822
US 1998-129570	B2	19980805
US 1998-137457	B2	19980820
US 1998-179605	B2	19981027
US 1999-261872	B2	19990303
US 1997-917023	A	19970822
US 1999-298490	A	19990423
US 1999-427768	A	19991027
WO 1999-US25234	W	19991027
US 2001-870838	B3	20010531

US 2001-871195 B3 20010531

OTHER SOURCE(S): MARPAT 135:318510

GI



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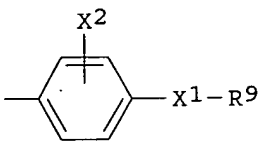
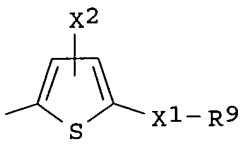


II

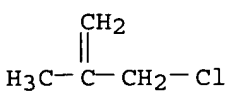


III

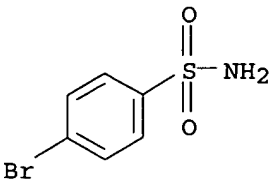
AB The title compds. [I; X = O, S, NR4, etc.; R4 = alkyl, alkenyl, cycloalkyl, etc.; R = H, alkyl, alkenyl, etc.; at least one of R1-R3 = II-III (wherein X1 = SO2, SO(NR10), SO, etc.; R9 = alkyl, alkenyl, alkynyl, etc.; X2 = H, halo, alkyl, etc.; R10 = H, alkyl, cycloalkyl); the remaining two of the groups of R1-R3 = H, OH, hydroxyalkyl, etc.] which are cyclooxygenase (COX) inhibitors, and in particular, are selective inhibitors of cyclooxygenase-2 (COX-2), and therefore are useful in treating pain, fever, inflammation, rheumatoid arthritis, and osteoarthritis, were prepared Thus, oxidation of 2-benzyl-4-(4-fluorophenyl)-5-[4-(methylthio)phenyl]-3(2H)-pyridazinone (preparation given) with MeCO3H in CH2Cl2 afforded 86% I [X = O; R = PhCH2; R1 = 4-FC6H4; R2 = 4-(MeSO2)C6H4; R3 = H], which showed IC50 of 0.014 μM against COX-2. COX-2 is the inducible isoform associated with inflammation, as opposed to the constitutive isoform, cyclooxygenase-1 (COX-1) which is an important "housekeeping" enzyme in many tissues, including the gastrointestinal (GI) tract and the kidneys. The selectivity of the compds. I for COX-2 minimizes the unwanted GI and renal side-effects seen with currently marketed non-steroidal anti-inflammatory drugs (NSAIDs).

IT **563-47-3**, 3-Chloro-2-methylpropene **701-34-8**, 4-Aminosulfonyl-1-bromobenzene
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reactant; preparation of arylpyridazinones as prostaglandin endoperoxide H synthase biosynthesis inhibitors)

RN 563-47-3 HCAPLUS
CN 1-Propene, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)



RN 701-34-8 HCAPLUS
CN Benzenesulfonamide, 4-bromo- (9CI) (CA INDEX NAME)

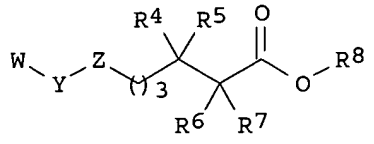


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 5 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:265252 HCAPLUS
DOCUMENT NUMBER: 134:295810
TITLE: Synthesis and use of substituted pyrrolidin-1-yl hexanoic acid derivatives as αvβ3 and αvβ5 integrin receptors
INVENTOR(S): Askew, Ben C.; Smith, Garry R.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 141 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2001024797	A1	20010412	WO 2000-US27033		20000929	<--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM						
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG						
CA 2386030	AA	20010412	CA 2000-2386030		20000929	<--
EP 1229910	A1	20020814	EP 2000-967201		20000929	<--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL						
JP 2003510360	T2	20030318	JP 2001-527796		20000929	
US 6413955	B1	20020702	US 2000-677677		20001002	<--
PRIORITY APPLN. INFO.:			US 1999-157490P	P	19991004	
			WO 2000-US27033	W	20000929	

OTHER SOURCE(S): MARPAT 134:295810
GI



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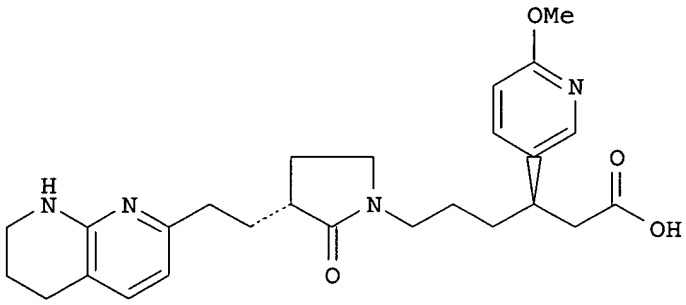


II

AB Compds. of formula I [wherein; W is a 5 or 6 membered monocyclic (aromatic) ring having 1-4 heteroatoms (N, O or S) wherein the ring nitrogen atoms are unsubstituted or substituted with 1 or 2 R1 groups, or a 9-14 membered polycyclic ring system, wherein the polycyclic ring system has 1-4 heteroatoms (N, O or S) in which the N atoms are substituted as described above; Y is (CH2)m, (CH2)m-(O, NR2 or S(O)0-2)-(CH2)n, etc., where any CH2 can be substituted with 1 or 2 R3 groups, m is 0-3 and n is 0-3; Z is a 5-6 membered heterocyclic system having 1-3 heteroatoms (N, O or S) optionally substituted with one or more R9 group and when 2 R9 substituents are on the same C-atom, they are taken together to form a C3-C6 cycloalkyl group; R1 is H, halo, (cyclo)alkyl, cycloheteroalkyl, aryl(alkyl), amino(alkyl), etc.; R2 is H, alkyl, aryl(alkyl), aminocarbonyl, cycloalkyl, aminoalkyl, etc.; R3 is H, alkyl, aryl(alkyl), halo, OH, oxo, CF3, etc.; R4 and R5 are H, alkyl, aryl(alkyl), halo, OH, alkylcarbonylamino, etc. or taken together the C-atom to form a CO; R6 and R7 are H, alkyl, aryl(alkyl), halo, OH, etc.; R8 is H, alkyl, aryl(alkyl), alkylcarbonyloxyalkyl, etc.; R9 is H, alkyl, aryl, halo, OH, etc.;]. Several examples of I are provided. For instance II was synthesized in 14 steps as a single enantiomer. Compds. I are antagonists of the integrin receptors αvβ3 and/or αvβ5. Compds. I were found to bind to human αvβ3 integrin with IC50 values less than 10 nM and to the αvβ5 integrin receptor with IC50 values less than 100 nM in competitive binding assays. A bone resorption-pit assay demonstrated the ability of compds. I to inhibit osteoclasts (bovine bone slices). Claimed uses for I are for inhibiting bone resorption, treating and preventing osteoporosis, inhibiting vascular restenosis, diabetic retinopathy, macular degeneration, angiogenesis, atherosclerosis, inflammatory arthritis, cancer, and metastatic tumor growth.

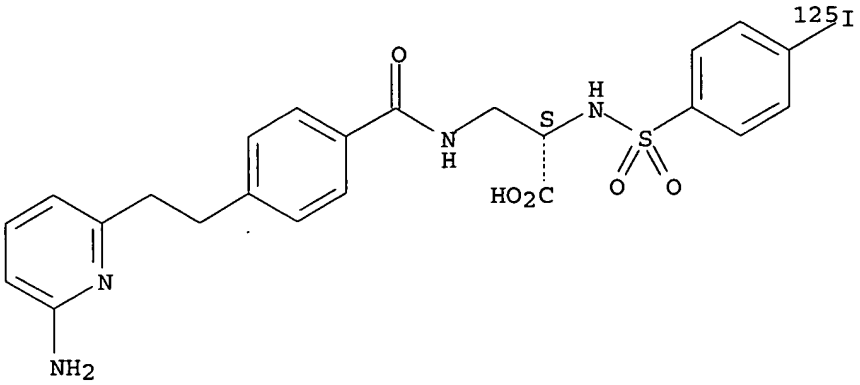
IT **204452-42-6P 312263-47-1P**
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation and use of substituted pyrrolidin-1-yl hexanoic acid derivs. as αvβ3 and αvβ5 integrin receptor antagonists)

RN 204452-42-6 HCAPLUS

CN L-Alanine, 3-[[4-[2-(6-amino-2-pyridinyl)ethyl]benzoyl]amino]-N-[[4-(iodo-

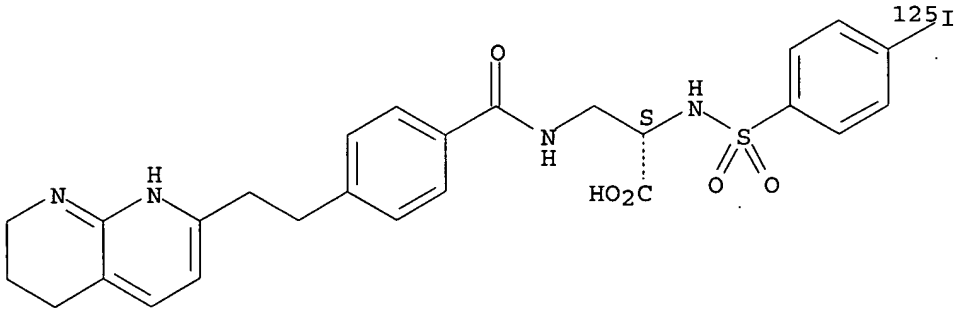
125I)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

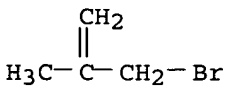


RN 312263-47-1 HCAPLUS
CN L-Alanine, N-[[4-(iodo-125I)phenyl]sulfonyl]-3-[[4-[2-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)ethyl]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



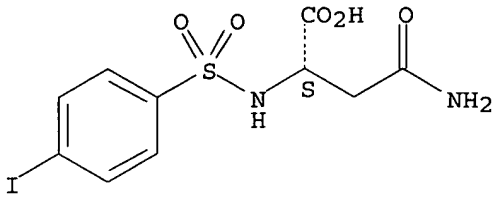
IT **1458-98-6**, 3-Bromo-2-methylpropene
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation and use of substituted pyrrolidin-1-yl hexanoic acid derivs. as αvβ3 and αvβ5 integrin receptor antagonists)
RN 1458-98-6 HCAPLUS
CN 1-Propene, 3-bromo-2-methyl- (9CI) (CA INDEX NAME)



IT **204452-34-6P 204452-35-7P 204452-36-8P**
204452-39-1P 204452-40-4P 312263-44-8P
312263-45-9P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and use of substituted pyrrolidin-1-yl hexanoic acid derivs. as αvβ3 and αvβ5 integrin receptor

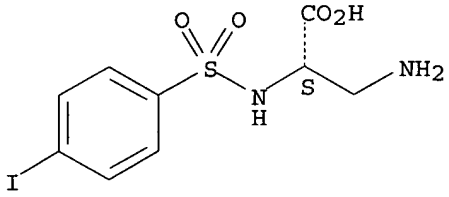
antagonists)
RN 204452-34-6 HCAPLUS
CN L-Asparagine, N2-[(4-iodophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



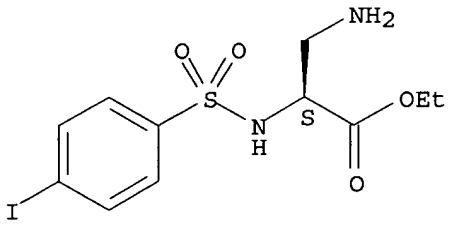
RN 204452-35-7 HCAPLUS
CN L-Alanine, 3-amino-N-[(4-iodophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204452-36-8 HCAPLUS
CN L-Alanine, 3-amino-N-[(4-iodophenyl)sulfonyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

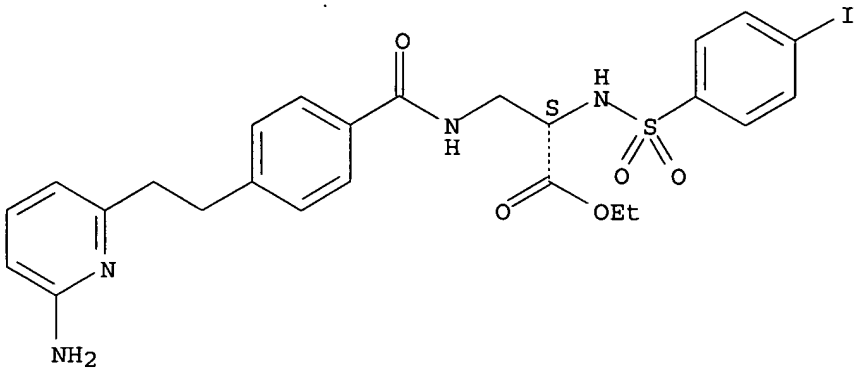
Absolute stereochemistry.



● HCl

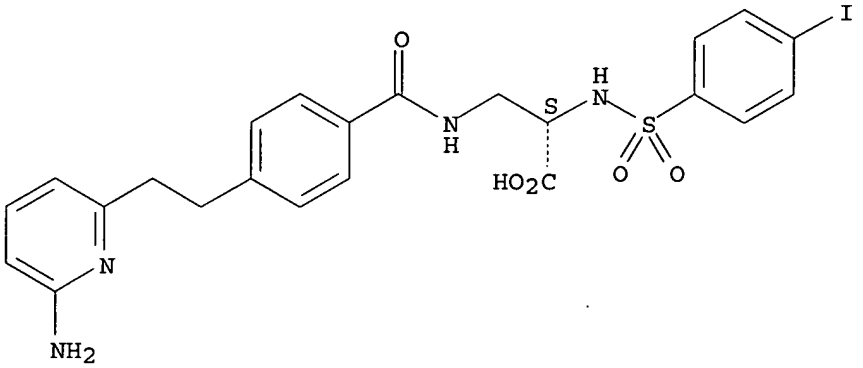
RN 204452-39-1 HCAPLUS
CN L-Alanine, 3-[[4-[2-(6-amino-2-pyridinyl)ethyl]benzoyl]amino]-N-[(4-iodophenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



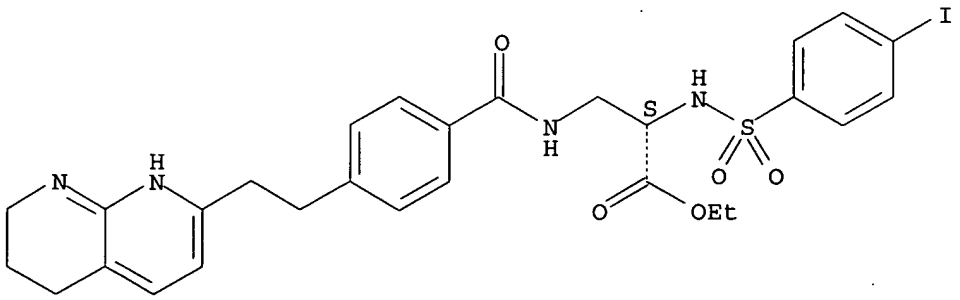
RN 204452-40-4 HCAPLUS
CN L-Alanine, 3-[[4-[2-(6-amino-2-pyridinyl)ethyl]benzoyl]amino]-N-[(4-iodophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



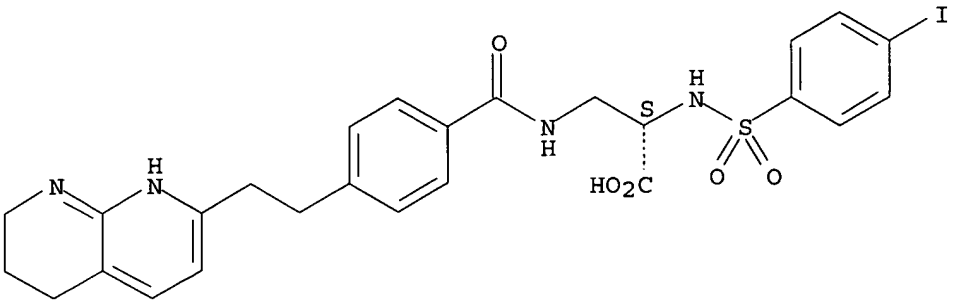
RN 312263-44-8 HCAPLUS
CN L-Alanine, N-[(4-iodophenyl)sulfonyl]-3-[[4-[2-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)ethyl]benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312263-45-9 HCAPLUS
CN L-Alanine, N-[(4-iodophenyl)sulfonyl]-3-[[4-[2-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)ethyl]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

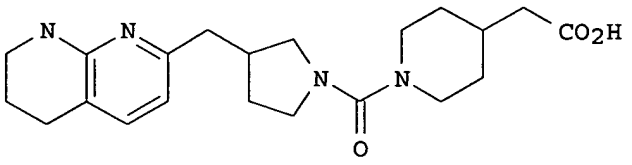


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 6 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:911080 HCAPLUS
DOCUMENT NUMBER: 134:56581
TITLE: Preparation of piperidinealkanoates as αv integrin antagonists
INVENTOR(S): Duggan, Mark E.; Hartman, George D.; Perkins, James J.; Ihle, Nathan
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000078317	A1	20001228	WO 2000-US16849		20000619 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2376077	AA	20001228	CA 2000-2376077		20000619 <--
EP 1194151	A1	20020410	EP 2000-942941		20000619 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
AU 748949	B2	20020613	AU 2000-57490		20000619 <--
JP 2003502373	T2	20030121	JP 2001-504380		20000619
US 6358970	B1	20020319	US 2000-599088		20000621 <--
PRIORITY APPLN. INFO.:			US 1999-140535P	P	19990623
			WO 2000-US16849	W	20000619

OTHER SOURCE(S): MARPAT 134:56581
GI



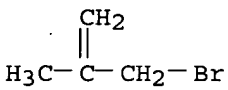
I

AB XYZCODECO2R5 [D = cycloalkylene, heterocyclylene, (hetero)arylene, etc.; E = bond, [(hetero)arylene- or heteroatom-interrupted or -terminated] alkylene, etc.; R5 = H, (ar)alkyl, aryl, etc.; X = (un)substituted amidino, -ureido, -heterocyclyl, -heteroaryl, etc.; Y = [(hetero)arylene- or heteroatom-interrupted or -terminated] alkylene; Z = n,1-azacycloalkylene; n = 2-7] were prepared as integrin receptor antagonists (no data). Thus, 3-(5,6,7,8-tetrahydro[1,8]naphthyridine-2-ylmethyl)pyrrolidine was condensed with Et piperidine-4-acetate hydrochloride (preparation each given) and COCl2 to give title compound I.

IT **1458-98-6**, 2-Bromomethylpropene
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation of piperidinealkanoates as αv integrin antagonists)

RN 1458-98-6 HCAPLUS

CN 1-Propene, 3-bromo-2-methyl- (9CI) (CA INDEX NAME)

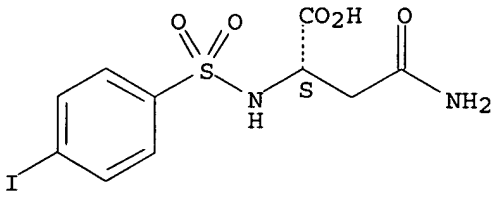


IT **204452-34-6P 204452-35-7P 204452-36-8P**
204452-39-1P 204452-40-4P 312263-44-8P
312263-45-9P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperidinealkanoates as αv integrin antagonists)

RN 204452-34-6 HCAPLUS

CN L-Asparagine, N2-[(4-iodophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

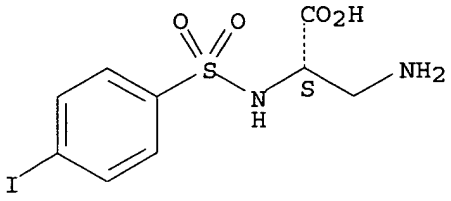
Absolute stereochemistry.



RN 204452-35-7 HCAPLUS

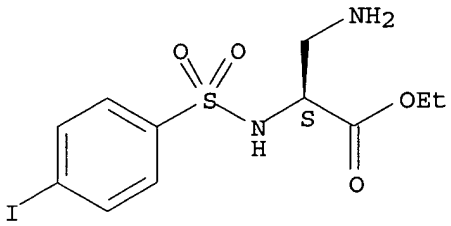
CN L-Alanine, 3-amino-N-[(4-iodophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204452-36-8 HCAPLUS
CN L-Alanine, 3-amino-N-[(4-iodophenyl)sulfonyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

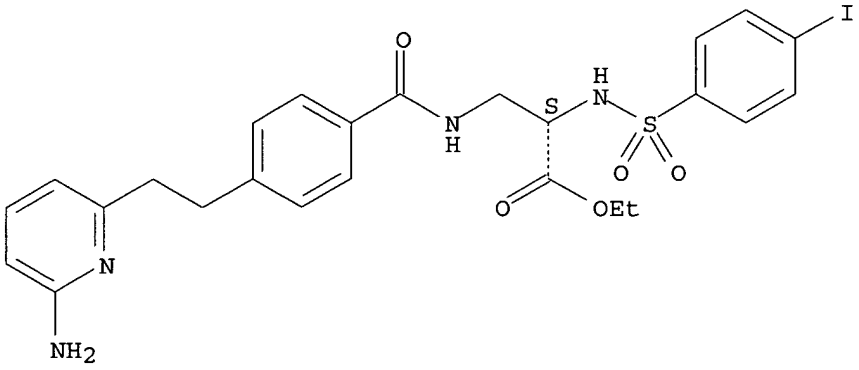
Absolute stereochemistry.



● HCl

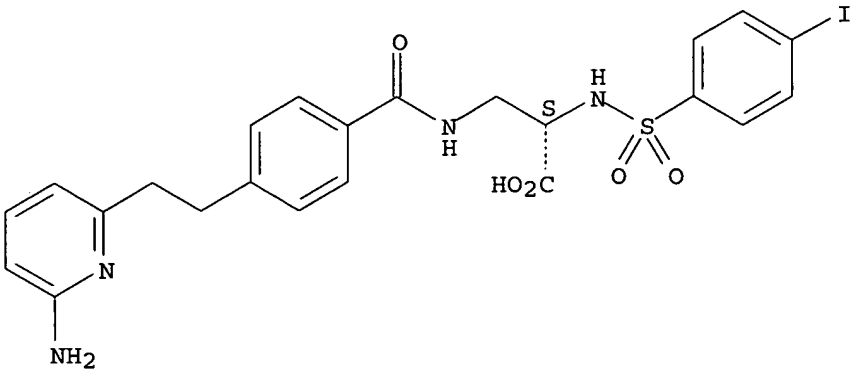
RN 204452-39-1 HCAPLUS
CN L-Alanine, 3-[[4-[2-(6-amino-2-pyridinyl)ethyl]benzoyl]amino]-N-[(4-iodophenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



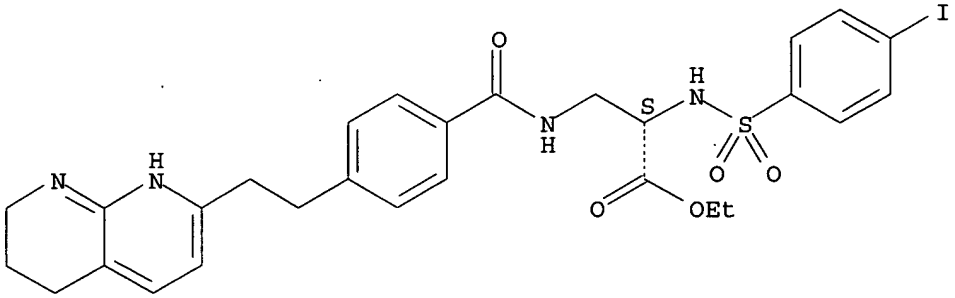
RN 204452-40-4 HCAPLUS
CN L-Alanine, 3-[[4-[2-(6-amino-2-pyridinyl)ethyl]benzoyl]amino]-N-[(4-iodophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



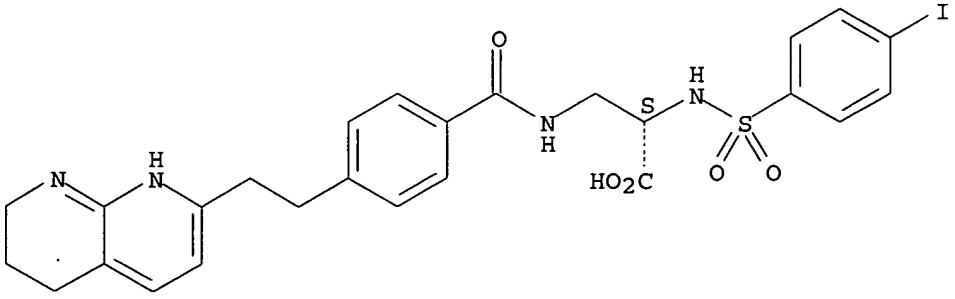
RN 312263-44-8 HCAPLUS
CN L-Alanine, N-[(4-iodophenyl)sulfonyl]-3-[[4-[2-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)ethyl]benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312263-45-9 HCAPLUS
CN L-Alanine, N-[(4-iodophenyl)sulfonyl]-3-[[4-[2-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)ethyl]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



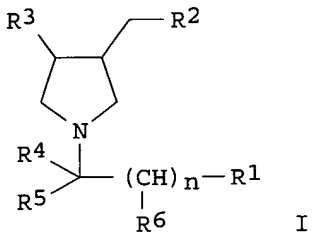
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 7 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:725459 HCAPLUS

DOCUMENT NUMBER: 133:296373
TITLE: Preparation of 3-phenyl-4-(heterocyclylmethyl)pyrrolidine modulators of chemokine receptor activity
INVENTOR(S): Caldwell, Charles; Chapman, Kevin; Hale, Jeffrey; Kim, Dooseop; Lynch, Christopher; Maccoss, Malcolm; Mills, Sander G.; Willoughby, Christopher; Berk, Scott; Kim, Ronald M.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: PCT Int. Appl., 202 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000059498	A1	20001012	WO 2000-US9074	20000405 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6498161	B1	20021224	US 2000-543019	20000404
PRIORITY APPLN. INFO.:			US 1999-128172P P	19990406

OTHER SOURCE(S): MARPAT 133:296373
GI



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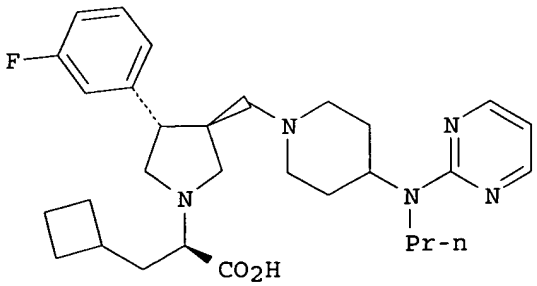


II

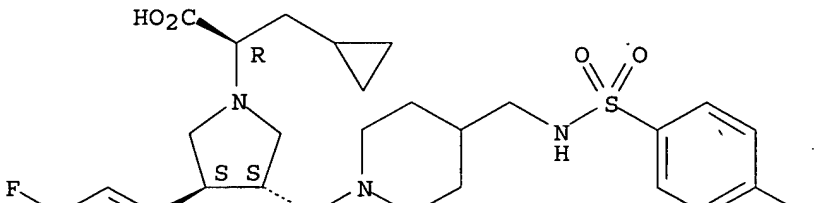
AB The title compds. (I) [wherein R1 = CO2H, NO2, tetrazolyl, hydroxyisoxazole, SO2NH(alkyl)R9, or PO3H2; R9 = H, (cyclo)alkyl, benzyl, or (un)substituted phenyl; R2 = (un)substituted piperidinyl, tetrahydropyridinyl, piperazinyl, or 1-oxa-8-azaspiro[4.5]decyl; R3 = (un)substituted Ph or heterocyclyl; R4 = H or (un)substituted alkyl, (alkyl)cycloalkyl, alkenyl, alkynyl, Ph, alkylphenyl, naphthyl, biphenyl, heterocyclyl, cyclohexenyl, etc.; R5 and R6 = independently H or (un)substituted alkyl; or R4 and R5 may be joined together to form an (un)substituted C3-8 cycloalkyl ring; n = 1-3] were prepared as modulators of chemokine receptors, especially the chemokine receptors CCR-5 and/or CCR-3. For example, 2-(R)-((3-(R)-formyl)-4-(S)-3-fluorophenylpyrrolidinyl-1-yl)-3-cyclobutanepropionic acid benzyl ester (preparation given) was treated with Pd/C and dissolved in ClCH2CH2Cl. 4-[N-(pyrimid-2-yl)-N-(prop-1-yl)amino]piperidine•HCl (4-step preparation given), NaBH(OAc)3, and TEA were added, followed by di-tert-butyldicarbonate, to give II. I showed binding activity to the CCR-5 or the CCR-3 receptor, generally with IC50 values of < 1 μM. The present invention is directed to compds. which inhibit the entry of human immunodeficiency virus (HIV) into target cells and are of value in the prevention and treatment of HIV infection and the resulting AIDS syndrome (no data). The invention is further directed to compds. which are useful in the prevention or treatment of certain inflammatory and immunoregulatory disorders, including asthma, allergic rhinitis, dermatitis, conjunctivitis, rheumatoid arthritis, and atherosclerosis (no data).

IT **301224-91-9P 301224-98-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3-phenyl-4-(heterocyclylmethyl)pyrrolidine chemokine receptor modulators by reaction of 3-phenyl-4-formylpyrrolidines with heterocycles)

RN 301224-91-9 HCAPLUS

CN 1-Pyrrolidineacetic acid, α-(cyclopropylmethyl)-3-(3-fluorophenyl)-4-[[4-[[[(4-fluorophenyl)sulfonyl]amino]methyl]-1-piperidinyl]methyl]-, (αR,3S,4S)- (9CI) (CA INDEX NAME)

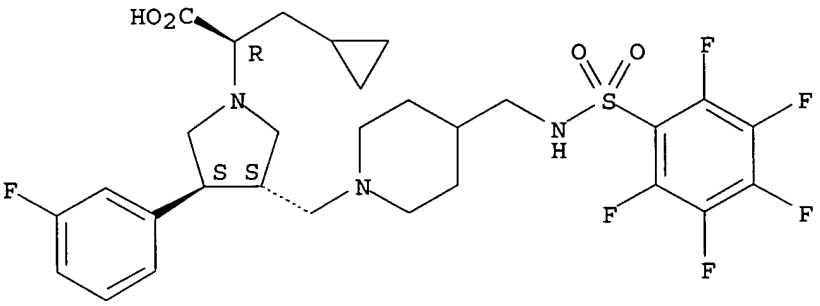
Absolute stereochemistry.



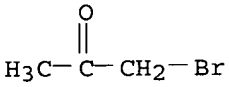
RN 301224-98-6 HCAPLUS

CN 1-Pyrrolidineacetic acid, α-(cyclopropylmethyl)-3-(3-fluorophenyl)-4-[[4-[[[(pentafluorophenyl)sulfonyl]amino]methyl]-1-piperidinyl]methyl]-, (αR,3S,4S)- (9CI) (CA INDEX NAME)

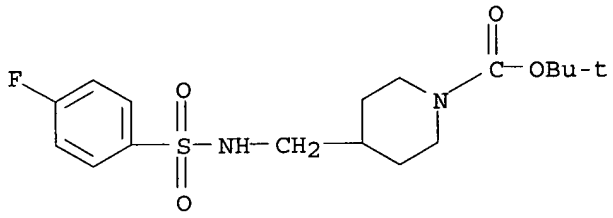
Absolute stereochemistry.



IT **598-31-2**, Bromoacetone
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation of 3-phenyl-4-(heterocyclylmethyl)pyrrolidine chemokine receptor modulators by reaction of 3-phenyl-4-formylpyrrolidines with heterocycles)
RN 598-31-2 HCAPLUS
CN 2-Propanone, 1-bromo- (8CI, 9CI) (CA INDEX NAME)



IT **301226-37-9P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenyl-4-(heterocyclylmethyl)pyrrolidine chemokine receptor modulators by reaction of 3-phenyl-4-formylpyrrolidines with heterocycles)
RN 301226-37-9 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[[(4-fluorophenyl)sulfonyl]amino]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 8 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:291005 HCAPLUS
DOCUMENT NUMBER: 132:321867
TITLE: Preparation of arylpyridazinones as prostaglandin endoperoxide H synthase biosynthesis inhibitors
INVENTOR(S): Black, Lawrence A.; Basha, Anwer; Kolasa, Teodozyj; Kort, Michael E.; Liu, Huaqing; Mccarty, Catherine M.; Patel, Meena V.; Rohde, Jeffrey J.; Coghlan, Michael

J.; Stewart, Andrew O.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 477 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

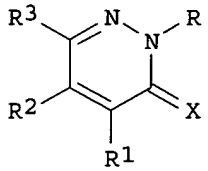
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000024719	A1	20000504	WO 1999-US25234	19991027 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2347982	AA	20000504	CA 1999-2347982	19991027 <--
AU 9965230	A1	20000515	AU 1999-65230	19991027 <--
AU 773237	B2	20040520		
EP 1124804	A1	20010822	EP 1999-953259	19991027 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6307047	B1	20011023	US 1999-427768	19991027 <--
BR 9914858	A	20020205	BR 1999-14858	19991027 <--
JP 2003512292	T2	20030402	JP 2000-578289	19991027
ZA 2001003310	A	20020723	ZA 2001-3310	20010423 <--
NO 2001002061	A	20010627	NO 2001-2061	20010426 <--
BG 105523	A	20011231	BG 2001-105523	20010519 <--

PRIORITY APPLN. INFO.:

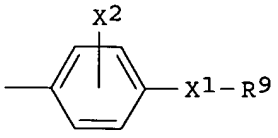
US 1998-179605	A	19981027
US 1999-261872	A	19990303
US 1999-298490	A	19990423
US 1999-427768	A	19991027
US 1997-56733P	P	19970822
US 1998-129570	B2	19980805
US 1998-137457	B2	19980820
WO 1999-US25234	W	19991027

OTHER SOURCE(S): MARPAT 132:321867

GI



I



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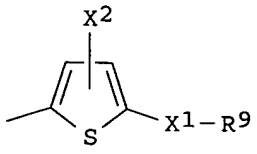
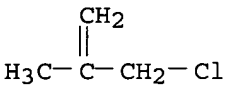


III

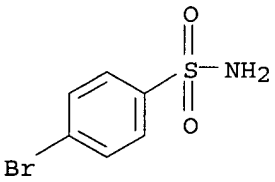
AB The title compds. [I; X = O, S, NR4, etc.; R4 = alkyl, alkenyl, cycloalkyl, etc.; R = H, alkyl, alkenyl, etc.; at least one of R1-R3 = II-III (wherein X1 = SO2, SO(NR10), SO, etc.; R9 = alkyl, alkenyl, alkynyl, etc.; X2 = H, halo, alkyl, etc.; R10 = H, alkyl, cycloalkyl); the remaining two of the groups of R1-R3 = H, OH, hydroxyalkyl, etc.] which are cyclooxygenase (COX) inhibitors, and in particular, are selective inhibitors of cyclooxygenase-2 (COX-2), and therefore are useful in treating pain, fever, inflammation, rheumatoid arthritis, osteoarthritis, adhesions, and cancer, were prepared Thus, oxidation of 2-benzyl-4-(4-fluorophenyl)-5-[4-(methylthio)phenyl]-3(2H)-pyridazinone (preparation given) with MeCO3H in CH2Cl2 afforded 86% I [X = O; R = PhCH2; R1 = 4-FC6H4; R2 = 4-(MeSO2)C6H4; R3 = H], which showed 0.014 μM against COX-2. COX-2 is the inducible isoform associated with inflammation, as opposed to the constitutive isoform, cyclooxygenase-1 (COX-1) which is an important "housekeeping" enzyme in many tissues, including the gastrointestinal (GI) tract and the kidneys. The selectivity of the compds. I for COX-2 minimizes the unwanted GI and renal side-effects seen with currently marketed non-steroidal anti-inflammatory drugs (NSAIDs).

IT **563-47-3**, 3-Chloro-2-methylpropene **701-34-8**, 4-Aminosulfonyl-1-bromobenzene
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reactant; preparation of arylpyridazinones as prostaglandin endoperoxide H synthase biosynthesis inhibitors)

RN 563-47-3 HCAPLUS
CN 1-Propene, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)



RN 701-34-8 HCAPLUS
CN Benzenesulfonamide, 4-bromo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

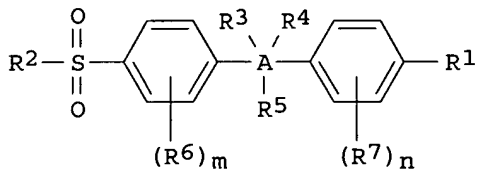
L47 ANSWER 9 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:795808 HCAPLUS
DOCUMENT NUMBER: 132:35714
TITLE: Preparation of heterocyclyl sulfonylbenzene compounds as anti-inflammatory/analgesic agents.
INVENTOR(S): Ando, Kazuo; Kato, Tomoki; Kawai, Akiyoshi; Nonomura, Tomomi
PATENT ASSIGNEE(S): Pfizer Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 236 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9964415	A1	19991216	WO 1999-IB970	19990531 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9938414	A1	19991230	AU 1999-38414	19990531 <--
EP 1086097	A1	20010328	EP 1999-921043	19990531 <--
EP 1086097	B1	20040519		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2002517496	T2	20020618	JP 2000-553424	19990531 <--
AT 267196	E	20040615	AT 1999-921043	19990531
PT 1086097	T	20040831	PT 1999-921043	19990531
ES 2220060	T3	20041201	ES 1999-921043	19990531
ZA 9903897	A	20010104	ZA 1999-3897	19990610 <--
US 6294558	B1	20010925	US 1999-446049	19991215 <--
US 2002045654	A1	20020418	US 2001-841348	20010424 <--
US 6608095	B2	20030819		
US 2003225064	A1	20031204	US 2003-465767	20030618
US 6727238	B2	20040427		
US 2004157824	A1	20040812	US 2004-771861	20040203

PRIORITY APPLN. INFO.:	WO 1998-IB912	W	19980611
	WO 1999-IB970	W	19990531
	US 1999-446049	A3	19991215
	US 2001-841348	A3	20010424
	US 2003-465767	A3	20030618

OTHER SOURCE(S): MARPAT 132:35714
GI



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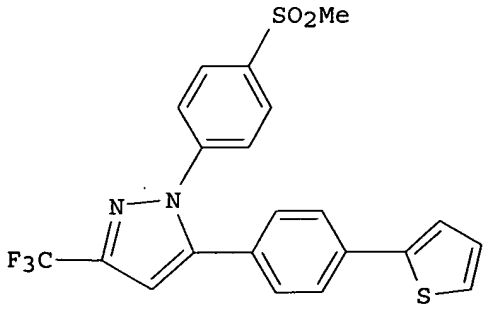


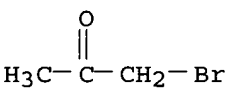
II

AB This invention provides a compound of formula (I) or its pharmaceutically acceptable salt thereof [wherein A is partially unsatd. or unsatd. five membered heterocyclic, or partially unsatd. or unsatd. five membered carbocyclic, wherein the 4-(sulfonyl)phenyl and the 4-substituted Ph in formula I are attached to ring atoms of Ring A, which are adjacent to each other; R1 is optionally substituted aryl or heteroaryl, with the proviso that when A is pyrazole, R1 is heteroaryl; R2 is C1-4 alkyl, halo-substituted C1-4 alkyl, C1-4 alkylamino, C1-4 dialkylamino or amino; R3, R4 and R5 are independently hydrogen, halo, C1-4 alkyl, halo-substituted C1-4 alkyl or the like; or two of R3, R4 and R5 are taken together with atoms to which they are attached and form a 4-7 membered ring; R6 and R7 are independently hydrogen, halo, C1-4 alkyl, halo-substituted C1-4 alkyl, C1-4 alkoxy, C1-4 alkylthio, C1-4 alkylamino or N,N-di C1-4 alkylamino; and m and n are independently 1, 2, 3 or 4]. This invention also provides a pharmaceutical composition useful for the treatment of a medical condition in which prostaglandins are implicated as pathogens. This invention relates to compound and pharmaceutical compns. for the treatment of cyclooxygenase mediated diseases. These compds. inhibit the biosynthesis of prostaglandins by intervention of the action of the enzyme cyclooxygenase on arachidonic acid, and are therefore useful in the treatment or alleviation of inflammation and other inflammation associated disorders, such as arthritis, in mammals (no data). Thus, To a stirred solution of 1-[4-(Methylsulfonyl)phenyl]-5-(4-bromophenyl)-3-trifluoromethyl-1H-pyrazole (0.27 g) in DME (8 mL) was added 3-thiophenboronic acid (0.09 g), bis(triphenylphosphine)palladium(II)chlor ide (0.05 g) and saturated NaHCO3 solution (2 mL) at room temperature under nitrogen.

The mixture was heated at reflux temperature for 16 h, and cooled down to room temperature to give, after purification by flash chromatog. eluting with Et acetate/hexane (1/1), 1-[4-(Methylsulfonyl)phenyl]-5-[4-(2-thienyl)phenyl]-3-trifluoromethyl-1H-pyrazole (II) in 64 % yield.

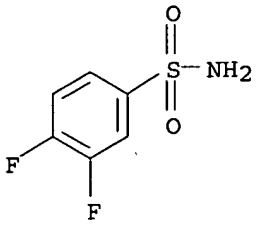
IT **598-31-2**, Bromoacetone
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation of heterocyclyl sulfonylbenzene compds. as cyclooxygenase inhibitors, prostaglandin biosynthesis inhibitors, anti-inflammatory, and analgesic agents)

RN 598-31-2 HCAPLUS
CN 2-Propanone, 1-bromo- (8CI, 9CI) (CA INDEX NAME)

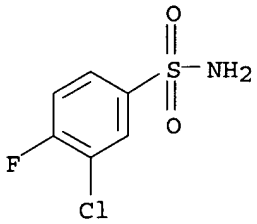


IT **108966-71-8P**, 3,4-Difluorobenzenesulfonamide **146533-46-2P**, 3-Chloro-4-fluorobenzenesulfonamide **252562-59-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclyl sulfonylbenzene compds. as cyclooxygenase inhibitors, prostaglandin biosynthesis inhibitors, anti-inflammatory, and analgesic agents)

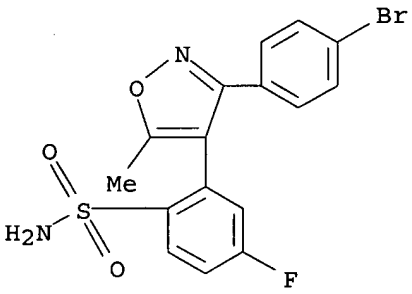
RN 108966-71-8 HCAPLUS
CN Benzenesulfonamide, 3,4-difluoro- (9CI) (CA INDEX NAME)



RN 146533-46-2 HCAPLUS
CN Benzenesulfonamide, 3-chloro-4-fluoro- (9CI) (CA INDEX NAME)



RN 252562-59-7 HCAPLUS
CN Benzenesulfonamide, 2-[3-(4-bromophenyl)-5-methyl-4-isoxazolyl]-4-fluoro- (9CI) (CA INDEX NAME)



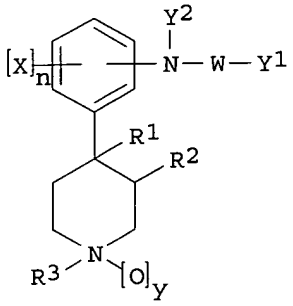
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 10 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:753211 HCAPLUS
DOCUMENT NUMBER: 132:3319
TITLE: Preparation of novel 4-phenylpiperidines for the treatment of pruritic dermatoses
INVENTOR(S): Armer, Richard Edward; Dutton, Christopher James; Gethin, David Morris; Gibson, Stephen Paul; Smith, Julian Duncan; Tommasini, Ivan
PATENT ASSIGNEE(S): Pfizer Inc., USA; Pfizer Limited
SOURCE: PCT Int. Appl., 171 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9959971	A1	19991125	WO 1999-IB886	19990517 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2332538	AA	19991125	CA 1999-2332538	19990517 <--
CA 2332538	C	19991125		
AU 9935312	A1	19991206	AU 1999-35312	19990517 <--
ZA 9903364	A	20001201	ZA 1999-3364	19990517 <--
BR 9910609	A	20010109	BR 1999-10609	19990517 <--
EP 1077940	A1	20010228	EP 1999-917038	19990517 <--
EP 1077940	B1	20040714		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2002515486	T2	20020528	JP 2000-549590	19990517 <--
AT 271038	E	20040715	AT 1999-917038	19990517
ES 2230846	T3	20050501	ES 1999-917038	19990517
US 2003078282	A1	20030424	US 2000-646255	20000511
US 6610711	B2	20030826		
PRIORITY APPLN. INFO.:			GB 1998-10671 A	19980518
			WO 1999-IB886 W	19990517

OTHER SOURCE(S): MARPAT 132:3319

GI



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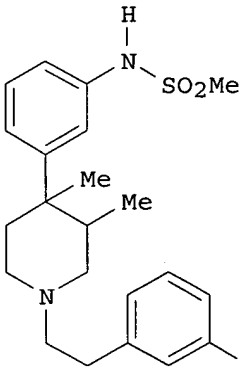


II

AB The title compds. [I; R1, R2 = H, alkyl; R3 = alkyl, alkenyl, alkynyl; W = SO2, CO, P(Y1):O, P(Y1):S; X = H, halo, alkyl, etc.; Y1 = alkyl, NH2, aryl, etc.; Y2 = H, alkyl, alkenyl, etc.; n = 0-2; yr = 0-1] and their pharmaceutically and veterinarily acceptable salts, useful for having utility in the treatment of pruritic dermatoses including allergic dermatitis and atopy in animals and humans, were prepared and formulated. E.g., synthesis of trans-3,4-dimethylpiperidine II which was found to display anti-pruritic activity when tested for its ability to inhibit the hind leg scratching behavior induced in male Wistar rats by the administration of the known pruritogenic agent, was given.

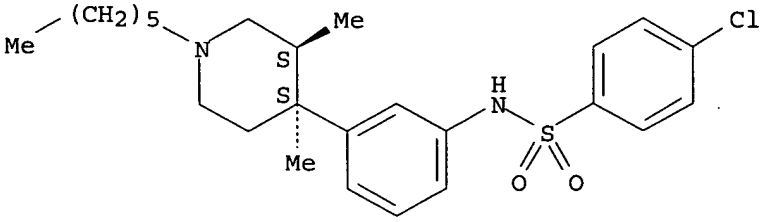
IT **250730-87-1P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel 4-phenylpiperidines for the treatment of pruritic dermatoses)

RN 250730-87-1 HCAPLUS

CN Benzenesulfonamide, 4-chloro-N-[3-[(3R,4R)-1-hexyl-3,4-dimethyl-4-piperidinyl]phenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

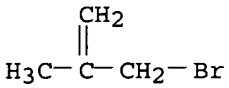


IT **1458-98-6 172376-41-9**

RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation of novel 4-phenylpiperidines for the treatment of pruritic dermatoses)

RN 1458-98-6 HCAPLUS

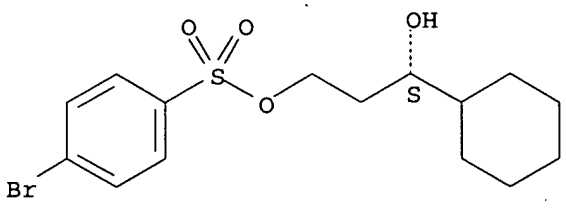
CN 1-Propene, 3-bromo-2-methyl- (9CI) (CA INDEX NAME)



RN 172376-41-9 HCAPLUS

CN Benzenesulfonic acid, 4-bromo-, (3S)-3-cyclohexyl-3-hydroxypropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

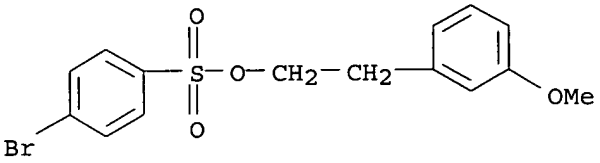


IT **32376-91-3P 93719-30-3P 250732-61-7P**
250732-63-9P 250732-66-2P 250732-67-3P
250732-69-5P 250732-71-9P

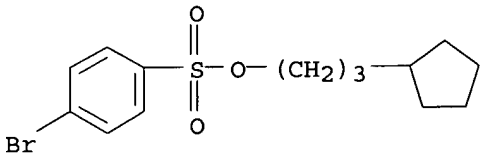
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel 4-phenylpiperidines for the treatment of pruritic dermatoses)

RN 32376-91-3 HCAPLUS

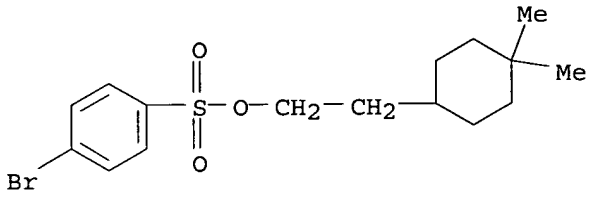
CN Benzenesulfonic acid, 4-bromo-, 2-(3-methoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)



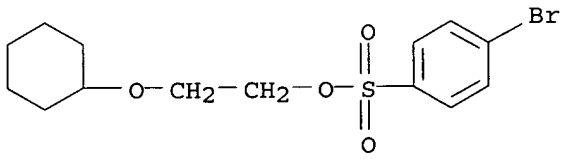
RN 93719-30-3 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 3-cyclopentylpropyl ester (9CI) (CA INDEX NAME)



RN 250732-61-7 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(4,4-dimethylcyclohexyl)ethyl ester (9CI) (CA INDEX NAME)



RN 250732-63-9 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(cyclohexyloxy)ethyl ester (9CI) (CA INDEX NAME)



RN 250732-66-2 HCAPLUS
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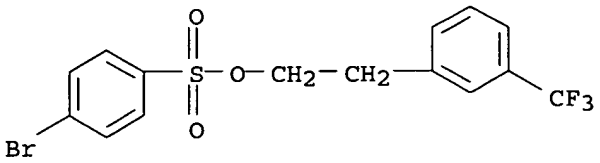
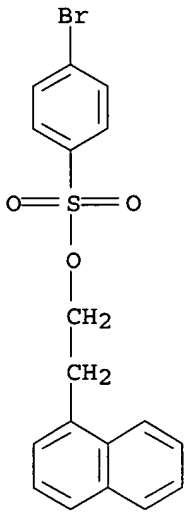
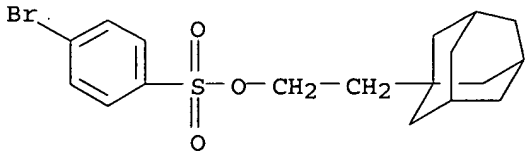


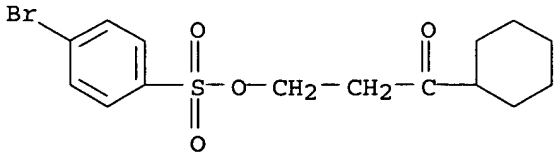
RN 250732-67-3 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(1-naphthalenyl)ethyl ester (9CI) (CA INDEX NAME)



RN 250732-69-5 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-tricyclo[3.3.1.13,7]dec-1-ylethyl ester (9CI) (CA INDEX NAME)



RN 250732-71-9 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 3-cyclohexyl-3-oxopropyl ester (9CI) (CA INDEX NAME)



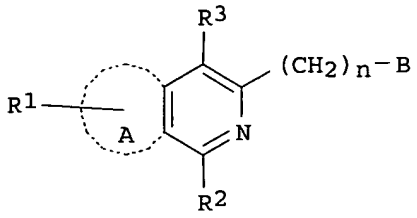
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 11 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:244638 HCAPLUS
DOCUMENT NUMBER: 130:311813
TITLE: Preparation of piperazinylisoquinolines and analogs as serotonin antagonists
INVENTOR(S): Ueno, Kohshi; Sasaki, Atsushi; Kawano, Koki; Okabe, Tadashi; Kitazawa, Noritaka; Takahashi, Keiko; Yamamoto, Noboru; Suzuki, Yuichi; Matsunaga, Manabu; Kubota, Atsuhiko
PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan
SOURCE: PCT Int. Appl., 740 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

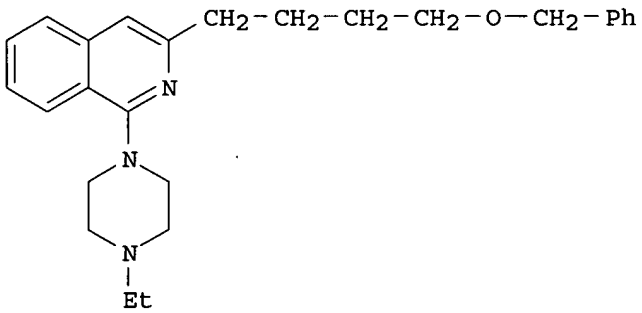
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9918077	A1	19990415	WO 1998-JP4465	19981002 <--
W: US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2000053647	A2	20000222	JP 1998-281752	19981002 <--
EP 1020445	A1	20000719	EP 1998-945593	19981002 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6340759	B1	20020122	US 2000-509778	20000331 <--
US 2002013460	A1	20020131	US 2001-852850	20010511 <--
US 6790844	B2	20040914		
US 2004204421	A1	20041014	US 2004-796673	20040310
US 6875761	B2	20050405		

PRIORITY APPLN. INFO.:	JP 1997-284290	A	19971002
	JP 1998-153416	A	19980602
	WO 1998-JP4465	W	19981002
	US 2000-509778	A3	20000331
	US 2001-852850	A3	20010511

OTHER SOURCE(S): MARPAT 130:311813
GI



I

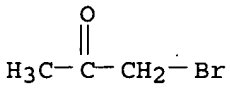


II

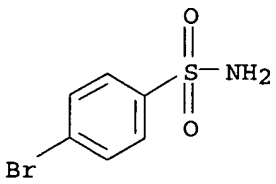
AB The title compds. I [ring A = benzene, pyridine, thiophene or furan ring; B = (un)substituted aryl, etc.; R1 = H, halo, etc.; R2 = 4-morpholinyl, etc.; R3 = H, halo, etc.; n = 0, or 1 - 6] are prepared I are central muscle relaxing drugs for treating, ameliorating or preventing spastic paralysis or ameliorating myotonia. In an in vitro test for 5HT1 receptor antagonism, the title compound II showed the Ki value of 21.2 nM.

IT **598-31-2**, 1-Bromo-2-propanone **701-34-8**
223557-22-0
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation of piperazinylisoquinolines and analogs as serotonin antagonists)

RN 598-31-2 HCAPLUS
CN 2-Propanone, 1-bromo- (8CI, 9CI) (CA INDEX NAME)

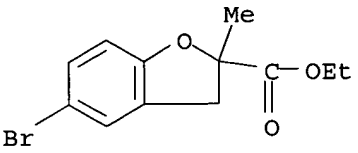


RN 701-34-8 HCAPLUS
CN Benzenesulfonamide, 4-bromo- (9CI) (CA INDEX NAME)



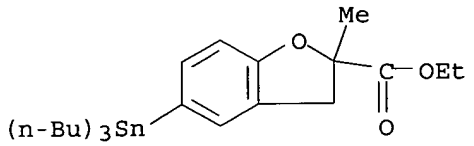
RN 223557-22-0 HCAPLUS

CN 2-Benzofurancarboxylic acid, 5-bromo-2,3-dihydro-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

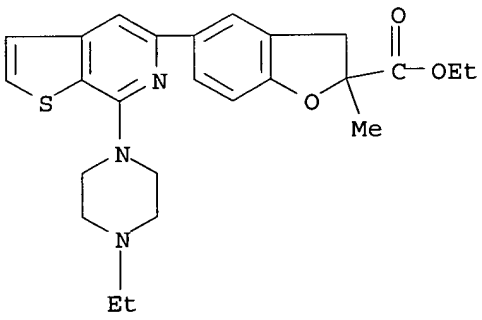


IT **223555-45-1P 223555-46-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperazinylisoquinolines and analogs as serotonin antagonists)

RN 223555-45-1 HCAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-2-methyl-5-(tributylstannyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 223555-46-2 HCAPLUS
CN 2-Benzofurancarboxylic acid, 5-[7-(4-ethyl-1-piperazinyl)thieno[2,3-c]pyridin-5-yl]-2,3-dihydro-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 12 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:166604 HCAPLUS
DOCUMENT NUMBER: 130:223284
TITLE: Preparation of arylpyridazinones as prostaglandin endoperoxide H synthase biosynthesis inhibitors
INVENTOR(S): Black, Lawrence A.; Basha, Anwer; Kolasa, Teodozyj; Kort, Michael E.; Liu, Huaqing; McCarty, Catherine M.; Patel, Meena V.; Rohde, Jeffrey J.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 307 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 9910331	A1	19990304	WO 1998-US16479		19980810	<--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM						
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG						
CA 2299300	AA	19990304	CA 1998-2299300		19980810	<--
AU 9886976	A1	19990316	AU 1998-86976		19980810	<--
AU 741317	B2	20011129				
EP 1007515	A1	20000614	EP 1998-938451		19980810	<--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO						
BR 9812127	A	20000718	BR 1998-12127		19980810	<--
TR 200000478	T2	20020422	TR 2000-200000478		19980810	<--
JP 2003516925	T2	20030520	JP 2000-507660		19980810	
ZA 9807555	A	19990223	ZA 1998-7555		19980820	<--
NO 2000000863	A	20000222	NO 2000-863		20000222	<--
NO 315423	B1	20030901				
MX 200001850	A	20001030	MX 2000-1850		20000222	<--
BG 104241	A	20001031	BG 2000-104241		20000315	<--
PRIORITY APPLN. INFO.:			US 1997-917023	A	19970822	
			US 1998-129570	A	19980805	
			WO 1998-US16479	W	19980810	

OTHER SOURCE(S): MARPAT 130:223284
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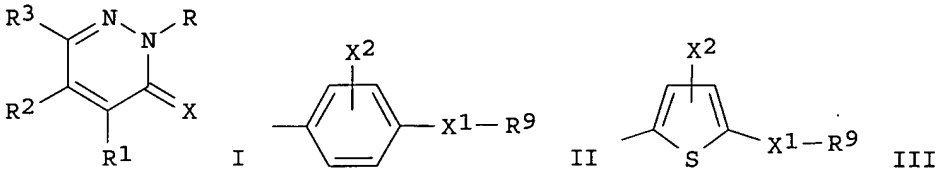
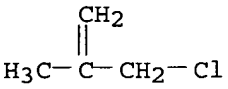


AB The title compds. [I; X = O, S, NR4, etc.; R4 = alkyl, alkenyl, cycloalkyl, etc.; R = H, alkyl, alkenyl, etc.; at least one of R1-R3 = II-III (wherein X1 = SO2, SO(NR10), SO, etc.; R9 = alkyl, alkenyl, alkynyl, etc.; X2 = H, halo, alkyl, etc.; R10 = H, alkyl, cycloalkyl); the remaining two of the groups of R1-R3 = H, OH, hydroxyalkyl, etc.] which are cyclooxygenase (COX) inhibitors, and in particular, are selective inhibitors of cyclooxygenase-2 (COX-2), and therefore are useful in treating pain, fever, inflammation, rheumatoid arthritis, osteoarthritis, adhesions, and cancer, were prepared Thus, oxidation of 2-benzyl-4-(4-fluorophenyl)-5-[4-(methylthio)phenyl]-3(2H)-pyridazinone (preparation given) with MeCO3H in CH2Cl2 afforded 86% I [X = O; R = PhCH2; R1 = 4-FC6H4; R2 = 4-(MeSO2)C6H4; R3 = H] which showed 0.014 μM against COX-2. COX-2 is the inducible isoform associated with inflammation, as opposed to the constitutive isoform, cyclooxygenase-1 (COX-1) which is an important

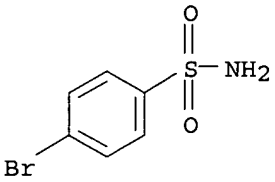
"housekeeping" enzyme in many tissues, including the gastrointestinal (GI) tract and the kidneys. The selectivity of the compds. I for COX-2 minimizes the unwanted GI and renal side-effects seen with currently marketed non-steroidal anti-inflammatory drugs (NSAIDs).

IT **563-47-3**, 3-Chloro-2-methylpropene **701-34-8**, 4-Aminosulfonyl-1-bromobenzene
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation of arylpyridazinones as prostaglandin endoperoxide H synthase biosynthesis inhibitors)

RN 563-47-3 HCAPLUS
CN 1-Propene, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)



RN 701-34-8 HCAPLUS
CN Benzenesulfonamide, 4-bromo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

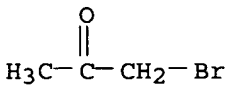
L47 ANSWER 13 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:686864 HCAPLUS
DOCUMENT NUMBER: 130:25035
TITLE: Fluorinated heterocycles: I. New 1,4-benzothiazines and 1,2,4-benzothiadiazines
AUTHOR(S): Vysokov, V. I.; Charushin, V. N.; Chupakhin, O. N.; Pashkevich, T. K.
CORPORATE SOURCE: Ural State Technical University, Yekaterinburg, 620002, Russia
SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (**1998**), 34(3), 428-433
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Chlorosulfonation of 3,4-difluoroaniline gave 2-amino-4,5-difluorobenzenesulfonyl chloride which was converted into the corresponding sulfonamide and sulfinic acid. The latter were used to synthesize various fluorine-containing 1,4-benzothiazine and 1,2,4-benzothiadiazine 1,1-dioxides.

IT **598-31-2**, Bromoacetone
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation of fluoro-substituted benzothiazine and benzothiadiazine dioxides)

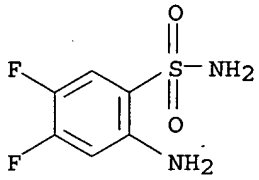
RN 598-31-2 HCAPLUS

CN 2-Propanone, 1-bromo- (8CI, 9CI) (CA INDEX NAME)

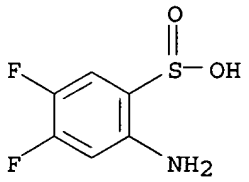


IT **1993-10-8P 152821-61-9P 216252-48-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluoro-substituted benzothiazine and benzothiadiazine dioxides)

RN 1993-10-8 HCAPLUS
CN Benzenesulfonamide, 2-amino-4,5-difluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)

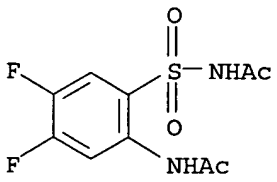


RN 152821-61-9 HCAPLUS
CN Benzenesulfinic acid, 2-amino-4,5-difluoro-, monosodium salt (9CI) (CA INDEX NAME)



● Na

RN 216252-48-1 HCAPLUS
CN Acetamide, N-[[2-(acetylamino)-4,5-difluorophenyl]sulfonyl]- (9CI) (CA INDEX NAME)

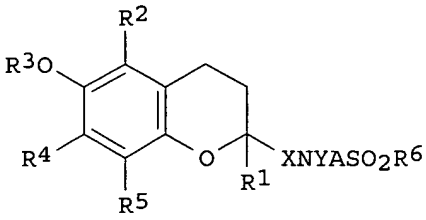


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 14 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:364966 HCAPLUS
DOCUMENT NUMBER: 129:27890
TITLE: Preparation of benzopyran derivatives and pharmaceutical compositions containing them
INVENTOR(S): Muller, Timothee; Moulin, Claudie; Duflos, Muriel; Robert-Piessard, Sylvie; Le Baut, Guillaume; Tonnerre, Alain; Caignard, Daniel-Henri; Manechez, Dominique; Renard, Pierre
PATENT ASSIGNEE(S): Adir Et Compagnie, Fr.
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
EP 844245	A1	19980527	EP 1997-402821	19971124	<--
EP 844245	B1	20010509			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
FR 2756284	A1	19980529	FR 1996-14470	19961126	<--
FR 2756284	B1	20000428			
AT 201020	E	20010515	AT 1997-402821	19971124	<--
ES 2157539	T3	20010816	ES 1997-402821	19971124	<--
PT 844245	T	20010928	PT 1997-402821	19971124	<--
CA 2222467	AA	19980526	CA 1997-2222467	19971125	<--
CA 2222467	C	20020528			
NO 9705402	A	19980527	NO 1997-5402	19971125	<--
CN 1183412	A	19980603	CN 1997-122919	19971125	<--
JP 10158260	A2	19980616	JP 1997-321858	19971125	<--
US 5889045	A	19990330	US 1997-977793	19971125	<--
BR 9705064	A	19990720	BR 1997-5064	19971125	<--
AU 9745383	A1	19980528	AU 1997-45383	19971126	<--
AU 720479	B2	20000601			
ZA 9710649	A	19980612	ZA 1997-10649	19971126	<--
GR 3036242	T3	20011031	GR 2001-401091	20010719	<--

PRIORITY APPLN. INFO.: FR 1996-14470 A 19961126
OTHER SOURCE(S): MARPAT 129:27890
GI



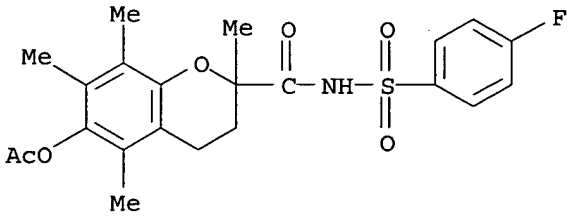
I

AB The title compds. I [R1 = alkyl, R2, R4, R5 = H, alkyl, R3 = H, alkyl, acyl, carboxyalkyl, alkoxycarbonyl, etc.; X = CO, CH2; Y = H, alkyl, aryl; A = bond, alkylphenyl; R6 = isocyanato, amino group, substituted urea,

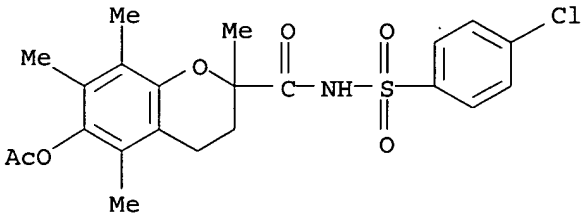
etc.] were prepared and their pharmacol. activity determined (no data). E.g., reaction of 6-acetoxy-3,4-dihydro-2,5,7,8-tetramethyl-1(2H)-benzopyran-2-carboxylic acid with MeSO2NH2 gave N-(6-acetoxy-3,4-dihydro-2,5,7,8-tetramethyl-1(2H)-benzopyran-2-carbonyl)methanesulfonamide.

IT **208039-12-7P 208039-13-8P 208039-14-9P**
208039-37-6P 208039-57-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and pharmacol. activity of benzopyran derivs.)

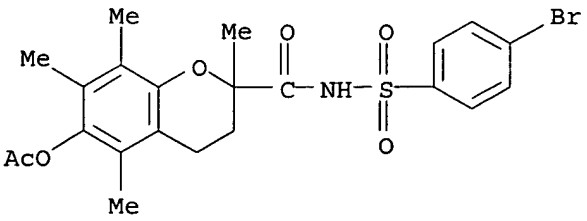
RN 208039-12-7 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, 6-(acetyloxy)-N-[(4-fluorophenyl)sulfonyl]-3,4-dihydro-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



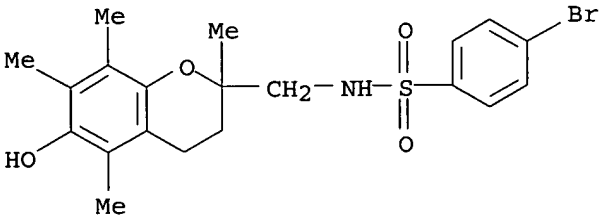
RN 208039-13-8 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, 6-(acetyloxy)-N-[(4-chlorophenyl)sulfonyl]-3,4-dihydro-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



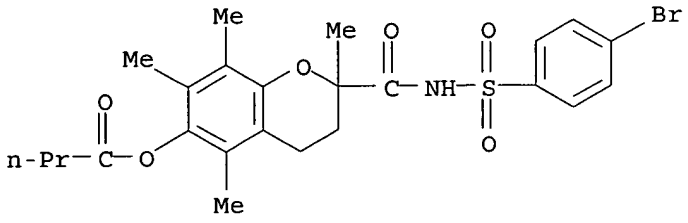
RN 208039-14-9 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, 6-(acetyloxy)-N-[(4-bromophenyl)sulfonyl]-3,4-dihydro-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



RN 208039-37-6 HCAPLUS
CN Benzenesulfonamide, 4-bromo-N-[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)methyl]- (9CI) (CA INDEX NAME)

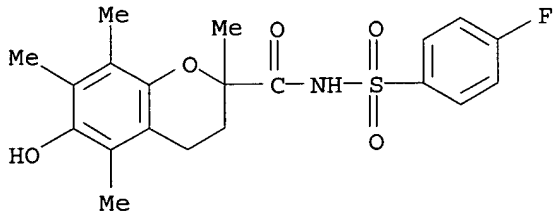


RN 208039-57-0 HCAPLUS
CN Butanoic acid, 2-[[[(4-bromophenyl)sulfonyl]amino]carbonyl]-3,4-dihydro-2,5,7,8-tetramethyl-2H-1-benzopyran-6-yl ester (9CI) (CA INDEX NAME)

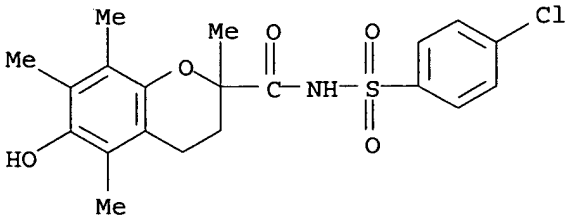


IT **208039-29-6P 208039-30-9P 208039-31-0P**
208039-36-5P 208039-39-8P 208039-46-7P
208039-47-8P 208039-49-0P 208039-50-3P
208039-51-4P 208039-56-9P 208039-62-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and pharmacol. activity of benzopyran derivs.)

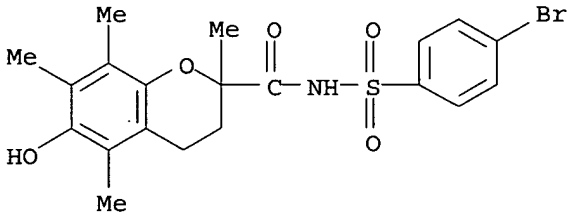
RN 208039-29-6 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, N-[(4-fluorophenyl)sulfonyl]-3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



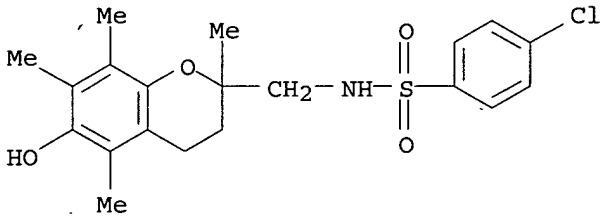
RN 208039-30-9 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, N-[(4-chlorophenyl)sulfonyl]-3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



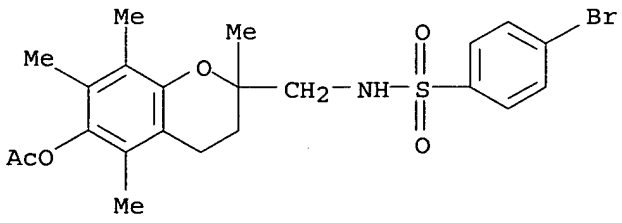
RN 208039-31-0 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, N-[(4-bromophenyl)sulfonyl]-3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



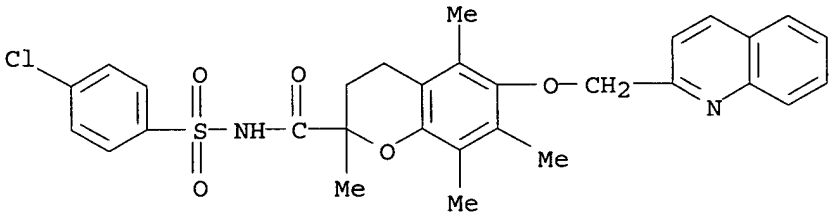
RN 208039-36-5 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)methyl]- (9CI) (CA INDEX NAME)



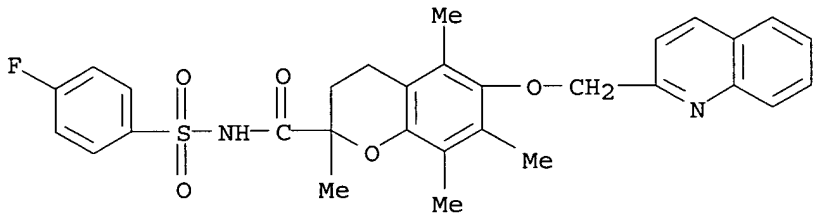
RN 208039-39-8 HCAPLUS
CN Benzenesulfonamide, N-[[6-(acetyloxy)-3,4-dihydro-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl]methyl]-4-bromo- (9CI) (CA INDEX NAME)



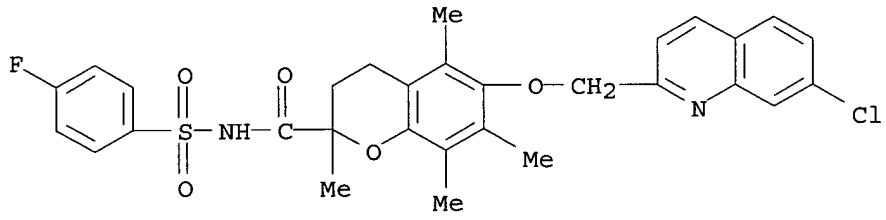
RN 208039-46-7 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, N-[(4-chlorophenyl)sulfonyl]-3,4-dihydro-2,5,7,8-tetramethyl-6-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)



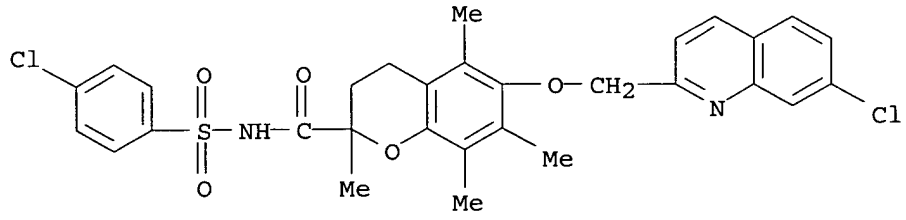
RN 208039-47-8 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, N-[(4-fluorophenyl)sulfonyl]-3,4-dihydro-2,5,7,8-tetramethyl-6-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)



RN 208039-49-0 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, 6-[(7-chloro-2-quinolinyl)methoxy]-N-[(4-fluorophenyl)sulfonyl]-3,4-dihydro-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)

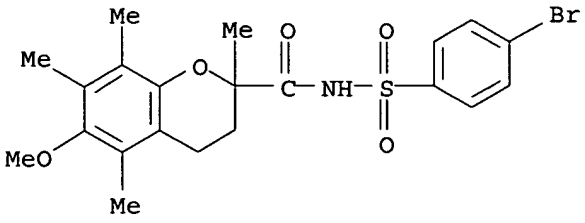


RN 208039-50-3 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, N-[(4-chlorophenyl)sulfonyl]-6-[(7-chloro-2-quinolinyl)methoxy]-3,4-dihydro-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)

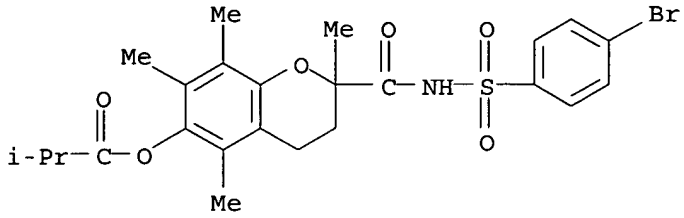


RN 208039-51-4 HCAPLUS
CN 2H-1-Benzopyran-2-carboxamide, N-[(4-bromophenyl)sulfonyl]-3,4-dihydro-6-

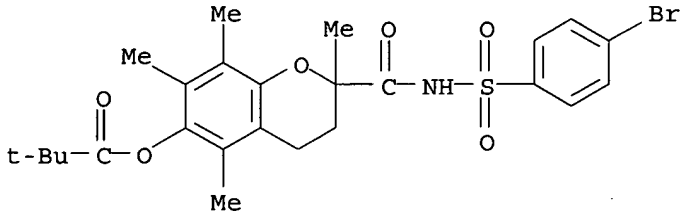
methoxy-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



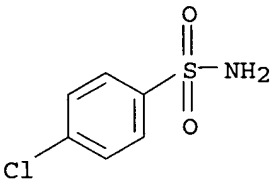
RN 208039-56-9 HCAPLUS
CN Propanoic acid, 2-methyl-, 2-[[[(4-bromophenyl)sulfonyl]amino]carbonyl]-3,4-dihydro-2,5,7,8-tetramethyl-2H-1-benzopyran-6-yl ester (9CI) (CA INDEX NAME)



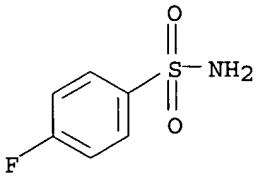
RN 208039-62-7 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-, 2-[[[(4-bromophenyl)sulfonyl]amino]carbonyl]-3,4-dihydro-2,5,7,8-tetramethyl-2H-1-benzopyran-6-yl ester (9CI) (CA INDEX NAME)



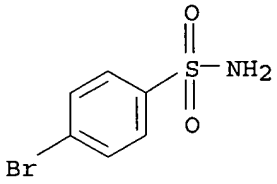
IT **98-64-6**, 4-Chlorobenzenesulfonamide **402-46-0**, 4-Fluorobenzenesulfonamide **701-34-8**, 4-Bromobenzenesulfonamide **106461-96-5 122005-20-3 208039-84-3 208039-86-5 208039-88-7 208039-90-1 208039-92-3 208039-94-5 208039-96-7**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(preparation and pharmacol. activity of benzopyran derivs.)
RN 98-64-6 HCAPLUS
CN Benzenesulfonamide, 4-chloro- (9CI) (CA INDEX NAME)



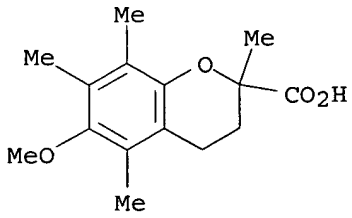
RN 402-46-0 HCAPLUS
CN Benzenesulfonamide, 4-fluoro- (9CI) (CA INDEX NAME)



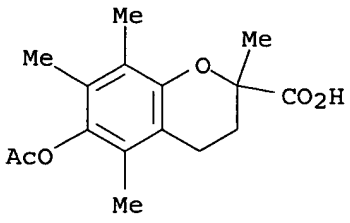
RN 701-34-8 HCAPLUS
CN Benzenesulfonamide, 4-bromo- (9CI) (CA INDEX NAME)



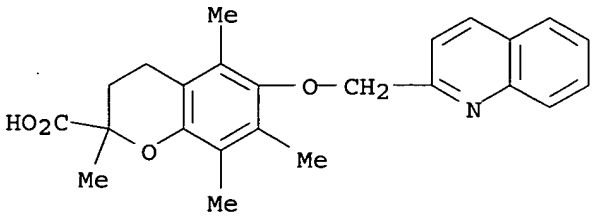
RN 106461-96-5 HCAPLUS
CN 2H-1-Benzopyran-2-carboxylic acid, 3,4-dihydro-6-methoxy-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



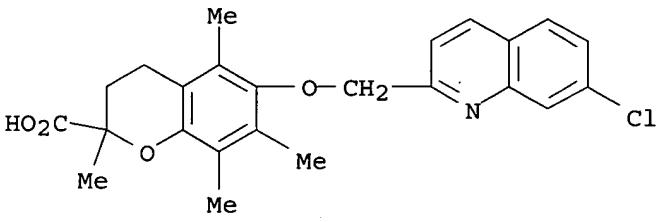
RN 122005-20-3 HCAPLUS
CN 2H-1-Benzopyran-2-carboxylic acid, 6-(acetyloxy)-3,4-dihydro-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



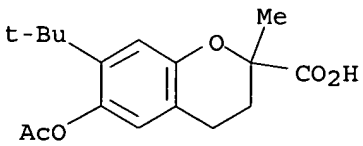
RN 208039-84-3 HCAPLUS
CN 2H-1-Benzopyran-2-carboxylic acid, 3,4-dihydro-2,5,7,8-tetramethyl-6-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)



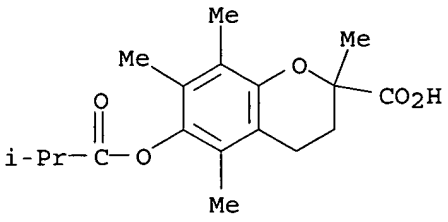
RN 208039-86-5 HCAPLUS
CN 2H-1-Benzopyran-2-carboxylic acid, 6-[(7-chloro-2-quinolinyl)methoxy]-3,4-dihydro-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



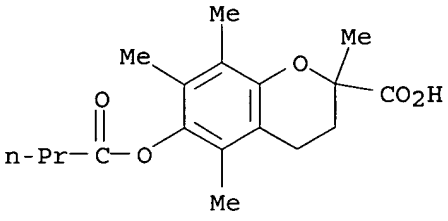
RN 208039-88-7 HCAPLUS
CN 2H-1-Benzopyran-2-carboxylic acid, 6-(acetyloxy)-7-(1,1-dimethylethyl)-3,4-dihydro-2-methyl- (9CI) (CA INDEX NAME)



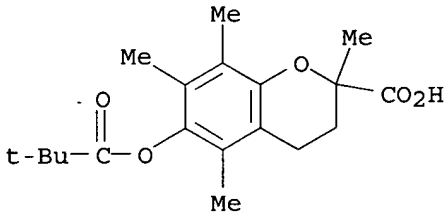
RN 208039-90-1 HCAPLUS
CN 2H-1-Benzopyran-2-carboxylic acid, 3,4-dihydro-2,5,7,8-tetramethyl-6-(2-methyl-1-oxopropoxy)- (9CI) (CA INDEX NAME)



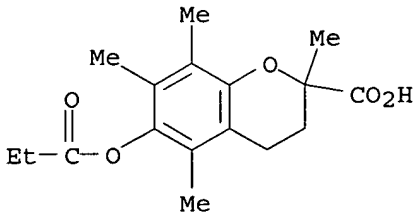
RN 208039-92-3 HCAPLUS
CN 2H-1-Benzopyran-2-carboxylic acid, 3,4-dihydro-2,5,7,8-tetramethyl-6-(1-oxobutoxy)- (9CI) (CA INDEX NAME)



RN 208039-94-5 HCAPLUS
CN 2H-1-Benzopyran-2-carboxylic acid, 6-(2,2-dimethyl-1-oxopropoxy)-3,4-dihydro-2,5,7,8-tetramethyl- (9CI) (CA INDEX NAME)



RN 208039-96-7 HCAPLUS
CN 2H-1-Benzopyran-2-carboxylic acid, 3,4-dihydro-2,5,7,8-tetramethyl-6-(1-oxopropoxy)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

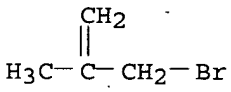
L47 ANSWER 15 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:784425 HCAPLUS
DOCUMENT NUMBER: 127:345953
TITLE: Deprotection of Allyl Groups with Sulfinic Acids and Palladium Catalyst
AUTHOR(S): Honda, Masanori; Morita, Hiromasa; Nagakura, Isao
CORPORATE SOURCE: Chemical Process Development Laboratory Drug Substance Manufacturing Plant, Pfizer Pharmaceuticals Inc., Taketoyo, 470-23, Japan
SOURCE: Journal of Organic Chemistry (**1997**), 62(25), 8932-8936
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:345953

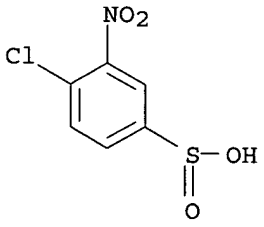
AB Sulfinic acids and their salts (e.g., PhSO2H, 4-MeC6H4SO2Na), together with a Pd catalyst [e.g., Pd(PPh3)4], were used to remove allylic groups from allylic esters, ethers, and amines. Excellent yields of the deprotected carboxylic acids, alcs., and amines were obtained.

IT **1458-98-6**, 3-Bromo-2-methylpropene **80917-26-6**, Benzenesulfinic acid, 4-chloro-3-nitro-, sodium salt
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(deprotection of allylic compds. with sulfinic acids and palladium catalyst)

RN 1458-98-6 HCAPLUS
CN 1-Propene, 3-bromo-2-methyl- (9CI) (CA INDEX NAME)



RN 80917-26-6 HCAPLUS
CN Benzenesulfinic acid, 4-chloro-3-nitro-, sodium salt (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 16 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1993:123849 HCAPLUS
DOCUMENT NUMBER: 118:123849
TITLE: Nucleophilic substitution reactions of methallyl arenesulphonates with anilines and

N,N-dimethylanilines

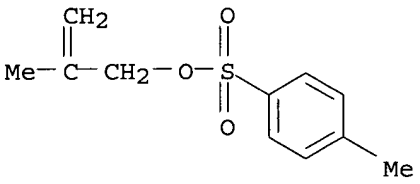
AUTHOR(S): Oh, Hyuck Keun; Shin, Chul Ho
CORPORATE SOURCE: Dep. Chem., Chonbuk Natl. Univ., Chonju, 560-756, S. Korea

SOURCE: Journal of Physical Organic Chemistry (**1992**), 5(11), 731-5
CODEN: JPOCEE; ISSN: 0894-3230
DOCUMENT TYPE: Journal
LANGUAGE: English

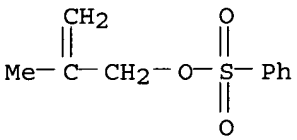
AB Kinetic studies of the reactions of CH2:CMeCH2OSO2C6H4Z-p (I; Z=Me,H,Cl,NO2) with anilines and N,N-dimethylanilines in acetonitrile at 45.0° are reported. The sign and magnitude of the cross-interaction consts. ρxz (and βxz) between substituents in the nucleophile (X) and leaving group (Z) suggest that the transition state (TS) is slightly tighter than that for the corresponding reactions of allyl arenesulfonates(II) . This is also supported by the observation that the magnitudes of ρx and ρz for I are uniformly greater than those for the reactions of II. These results are in line with the simple MO theory that the 2-position of the allyl system is inactive electronically. The steric effect of the 2-Me group in II causes a rate retardation and a shift of the TS toward a later position along the reaction coordinate with a slight increase in the overall tightness of the TS structure. The large |ρxz| value obtained eliminates the possibility of an SN2' mechanism.

IT **20443-62-3 20443-63-4 20443-64-5 77618-50-9**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(nucleophilic substitution reaction of, with anilines and dimethylanilines, kinetics and mechanism of)

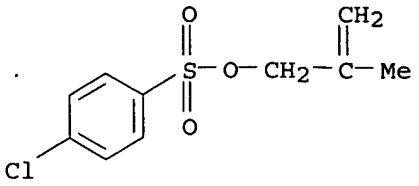
RN 20443-62-3 HCAPLUS
CN 2-Propen-1-ol, 2-methyl-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)



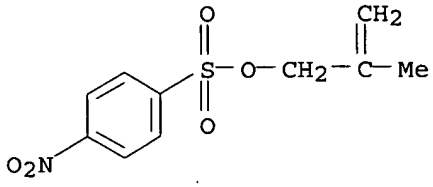
RN 20443-63-4 HCAPLUS
CN 2-Propen-1-ol, 2-methyl-, benzenesulfonate (7CI, 8CI, 9CI) (CA INDEX NAME)



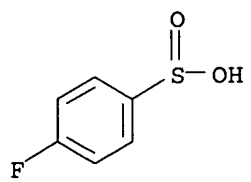
RN 20443-64-5 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-methyl-2-propenyl ester (9CI) (CA INDEX NAME)



RN 77618-50-9 HCAPLUS
CN Benzenesulfonic acid, 4-nitro-, 2-methyl-2-propenyl ester (9CI) (CA INDEX NAME)

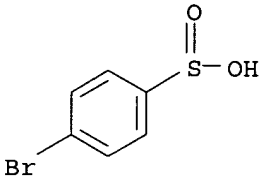


L47 ANSWER 17 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:118372 HCAPLUS
DOCUMENT NUMBER: 112:118372
TITLE: Hydration of 1- and 3-(arylsulfonyl)-1-propynes and (arylsulfonyl)allenes
AUTHOR(S): Mikhailova, V. N.; Bulat, A. D.; Yurevich, V. P.; Ezhova, L. A.
CORPORATE SOURCE: Leningr. Inst. Sov. Torgovly, Leningrad, USSR
SOURCE: Zhurnal Organicheskoi Khimii (**1988**), 24(9), 1948-52
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 112:118372
AB Reaction of isomeric RSO2CH2C.tplbond.CH (R = Ph, substituted Ph), RSO2CH:C:CH2 (R = Ph, 4-FC6H4, 4-MeC6H4, 4-O2NC6H4), and RSO2C:CMe (R = Ph, 4-FC6H4) with R1NH2 (R1 = 3-MeC6H4, 4-MeOC6H4) in an aqueous-organic solvent gives RSO2CH2COMe via the unstable enamine intermediates RSO2CH:CMeNHR1.
IT **369-51-7P 1195-33-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 369-51-7 HCAPLUS
CN Benzenesulfinic acid, 4-fluoro- (9CI) (CA INDEX NAME)

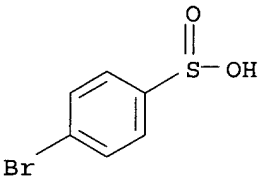


RN 1195-33-1 HCAPLUS

CN Benzenesulfinic acid, 4-bromo- (9CI) (CA INDEX NAME)



IT **34176-08-4**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(substitution reaction of, with bromoacetone)
RN 34176-08-4 HCAPLUS
CN Benzenesulfinic acid, 4-bromo-, sodium salt (9CI) (CA INDEX NAME)



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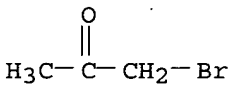
IT **598-31-2**, Bromoacetone
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(substitution reaction of, with sodium arylsulfinates)
RN 598-31-2 HCAPLUS
CN 2-Propanone, 1-bromo- (8CI, 9CI) (CA INDEX NAME)



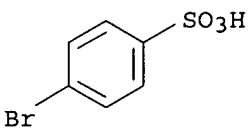
L47 ANSWER 18 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:45212 HCAPLUS
DOCUMENT NUMBER: 102:45212
TITLE: Stereochemistry of allyl sulfones. On the structure of metalated allyl sulfones and their stereochemistry of alkylation
AUTHOR(S): Trost, Barry M.; Schmuff, Norman R.
CORPORATE SOURCE: McElvain Lab. Org. Chem., Univ. Wisconsin, Madison, WI, 53706, USA
SOURCE: Journal of the American Chemical Society (**1985**), 107(2), 396-405
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:45212

AB Stereochem. studies involving alkylation of metalated allyl sulfones are probed to address the question of the structure of these important synthetic intermediates. In contrast to recent conclusions, both exptl. and theor., declaring sulfone-stabilized carbanions planar, the diastereoselectivity of these alkylations questions such conclusions even though the addnl. allylic conjugation would have been anticipated to provide a further driving force for planarity. A model to rationalize the seemingly contrasteric highly diastereoselective alkylations in which the sulfone-stabilized allylic carbanion exists as a somewhat pyramidalized organometallic emerges. The preferred conformations of the cyclohexenyl allylic sulfones place the sulfone moiety in an axial orientation and, in at least one acyclic case, the C-S bond parallel to the p-orbitals. An electronic stabilization is proposed to account for this conformation. In addition, the stereochem. of the palladium-catalyzed allylic alkylation with arylsulfinate places this nucleophile into the class of heteroatom nucleophiles that proceed with predominant net retention of configuration.

IT **5015-75-8**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction of, with carvyl acetate, catalyst for)

RN 5015-75-8 HCAPLUS

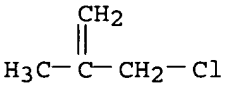
CN Benzenesulfonic acid, 4-bromo-, sodium salt (9CI) (CA INDEX NAME)



IT **563-47-3**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction of, with sodium benzenesulfinate)

RN 563-47-3 HCAPLUS

CN 1-Propene, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)



L47 ANSWER 19 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1985:5305 HCAPLUS

DOCUMENT NUMBER: 102:5305

TITLE: Substituent effect on the acetolysis of neophyl p-bromobenzenesulfonates

AUTHOR(S): Fujio, Mizue; Funatsu, Kimito; Shibata, Koji; Yoshinaga, Hironori; Maeda, Yasuyuki; Goto, Mutsuo; Mishima, Masaaki; Tsuno, Yuho

CORPORATE SOURCE: Fac. Sci., Kyushu Univ., Fukuoka, 812, Japan

SOURCE: Memoirs of the Faculty of Science, Kyushu University, Series C: Chemistry (**1984**), 14(2), 319-32
CODEN: MFKCAL; ISSN: 0085-2635

DOCUMENT TYPE: Journal

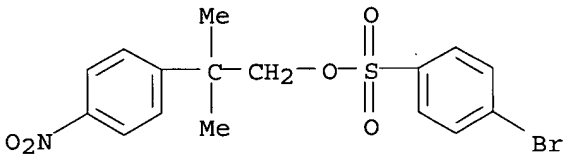
LANGUAGE: English

AB Substituent effects on acetolysis kinetics of several RC6H4CMe2CH2OBs (Bs = brosylate; R = p-MeO, p-MeS, m-Me, etc.), as well as of some analogous disubstituted derivs., were determined An r value (a measure of resonance demand) of 0.56 in the LArSR equation indicated that the mechanism involves a rate-determining aryl-assisted transition state, which cascades down to the tertiary carbonium ion without staying as a bridged intermediate. Thus, the substituent effect maybe viewed as the effect on the aryl-assisted ionization step. The application of the Brown ρσ+ equation is criticized.

IT **18755-55-0P 18755-58-3P 24517-38-2P**
28204-21-9P 83324-07-6P 83324-08-7P
83324-09-8P 83324-10-1P 83324-11-2P
83324-12-3P 83324-13-4P 83324-14-5P
83324-15-6P 83324-16-7P 83324-17-8P
83324-18-9P 83324-19-0P 83324-20-3P
93748-33-5P 93748-34-6P 93748-35-7P
93748-36-8P 93748-37-9P 93748-38-0P
93748-39-1P 93748-40-4P 93748-41-5P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetolysis of, kinetics of)

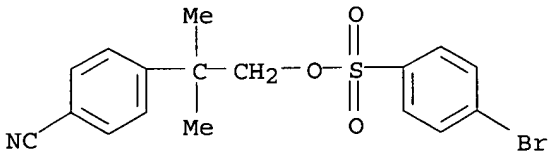
RN 18755-55-0 HCAPLUS

CN Benzenesulfonic acid, 4-bromo-, 2-methyl-2-(4-nitrophenyl)propyl ester (9CI) (CA INDEX NAME)



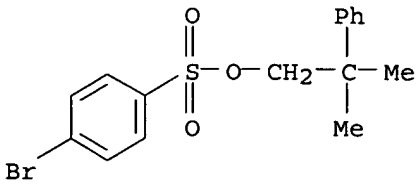
RN 18755-58-3 HCAPLUS

CN Benzenesulfonic acid, 4-bromo-, 2-(4-cyanophenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)

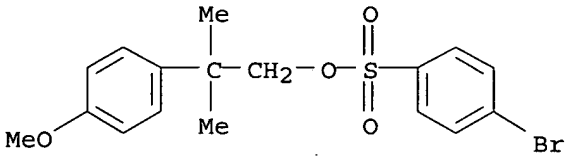


RN 24517-38-2 HCAPLUS

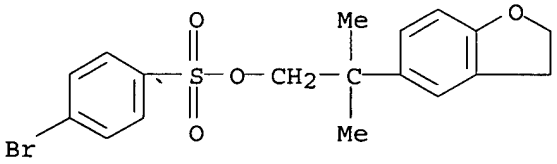
CN Benzenesulfonic acid, 4-bromo-, 2-methyl-2-phenylpropyl ester (9CI) (CA INDEX NAME)



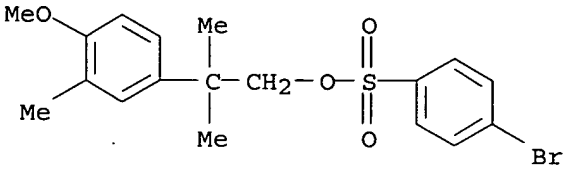
RN 28204-21-9 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(4-methoxyphenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



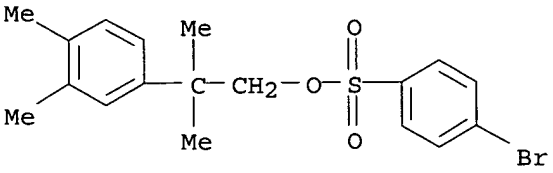
RN 83324-07-6 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(2,3-dihydro-5-benzofuranyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



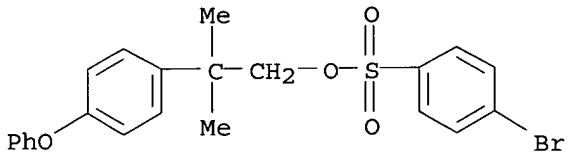
RN 83324-08-7 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(4-methoxy-3-methylphenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



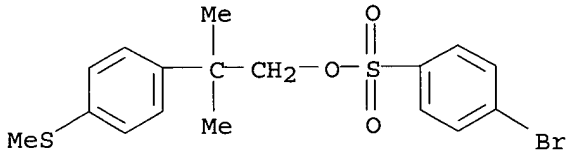
RN 83324-09-8 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(3,4-dimethylphenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



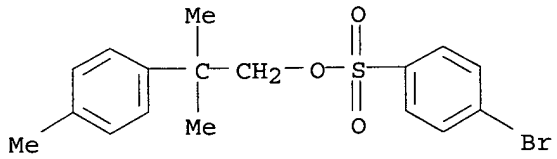
RN 83324-10-1 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-methyl-2-(4-phenoxyphenyl)propyl ester (9CI) (CA INDEX NAME)



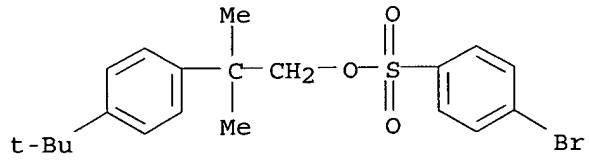
RN 83324-11-2 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-methyl-2-[4-(methylthio)phenyl]propyl ester (9CI) (CA INDEX NAME)



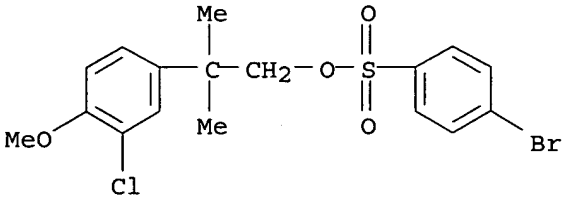
RN 83324-12-3 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-methyl-2-(4-methylphenyl)propyl ester (9CI) (CA INDEX NAME)



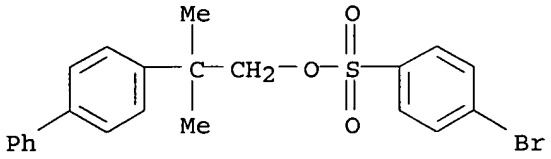
RN 83324-13-4 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-[4-(1,1-dimethylethyl)phenyl]-2-methylpropyl ester (9CI) (CA INDEX NAME)



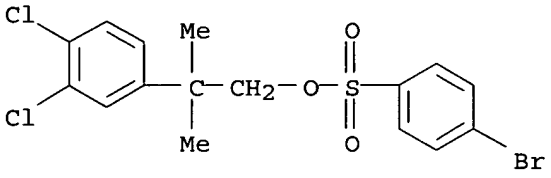
RN 83324-14-5 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(3-chloro-4-methoxyphenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



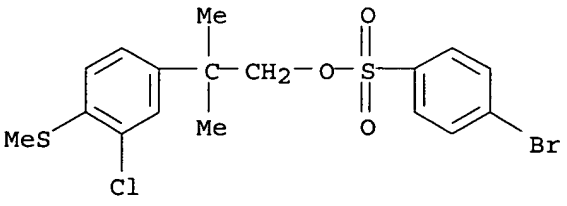
RN 83324-15-6 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-[1,1'-biphenyl]-4-yl-2-methylpropyl ester (9CI) (CA INDEX NAME)



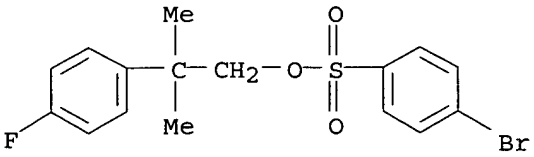
RN 83324-16-7 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(3,4-dichlorophenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



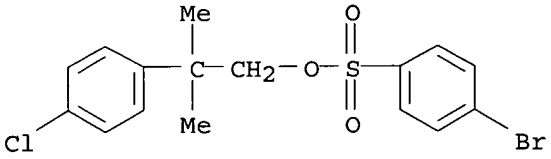
RN 83324-17-8 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-[3-chloro-4-(methylthio)phenyl]-2-methylpropyl ester (9CI) (CA INDEX NAME)



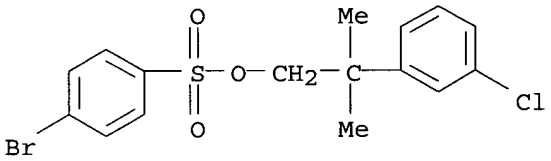
RN 83324-18-9 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(4-fluorophenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



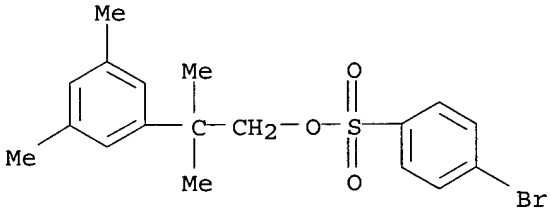
RN 83324-19-0 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(4-chlorophenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



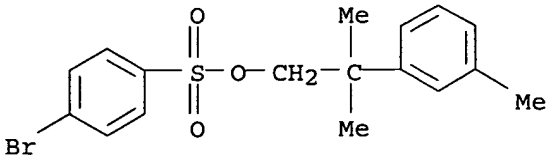
RN 83324-20-3 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(3-chlorophenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



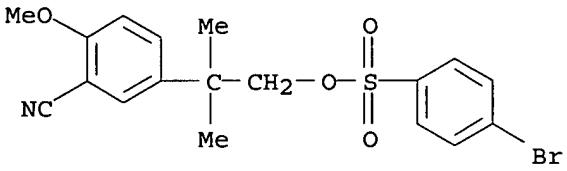
RN 93748-33-5 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(3,5-dimethylphenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



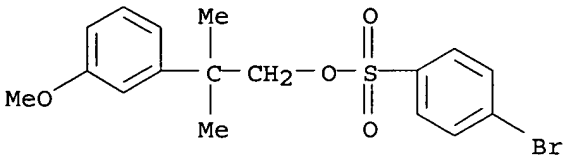
RN 93748-34-6 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-methyl-2-(3-methylphenyl)propyl ester (9CI) (CA INDEX NAME)



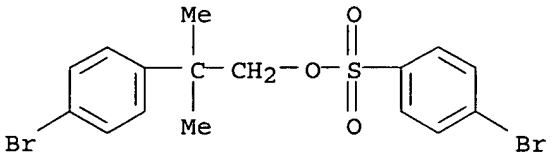
RN 93748-35-7 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(3-cyano-4-methoxyphenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



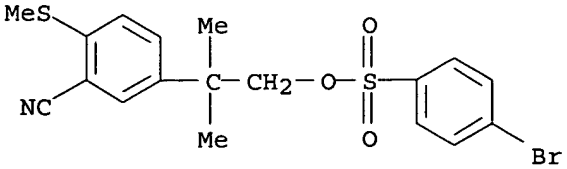
RN 93748-36-8 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(3-methoxyphenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



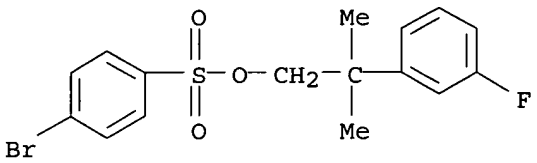
RN 93748-37-9 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(4-bromophenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



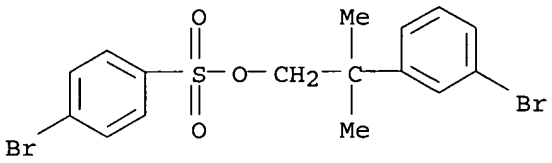
RN 93748-38-0 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-[3-cyano-4-(methylthio)phenyl]-2-methylpropyl ester (9CI) (CA INDEX NAME)



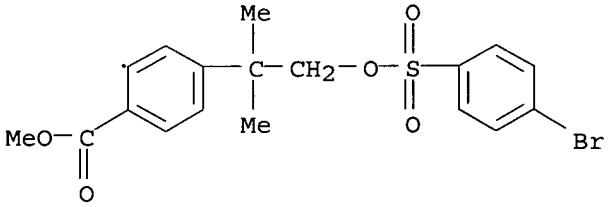
RN 93748-39-1 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(3-fluorophenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



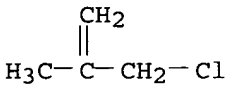
RN 93748-40-4 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-(3-bromophenyl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



RN 93748-41-5 HCAPLUS
CN Benzoic acid, 4-[2-[[(4-bromophenyl)sulfonyl]oxy]-1,1-dimethylethyl]-, methyl ester (9CI) (CA INDEX NAME)



IT **563-47-3**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction of, with chloroanisole in presence of carbon disulfide)
RN 563-47-3 HCAPLUS
CN 1-Propene, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)

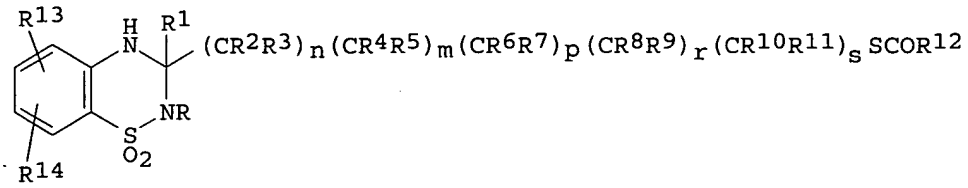


L47 ANSWER 20 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:582465 HCAPLUS
DOCUMENT NUMBER: 97:182465
TITLE: Benzothiadiazines having diuretic activity
INVENTOR(S): Haugwitz, Rudiger D.
PATENT ASSIGNEE(S): E. R. Squibb and Sons, Inc., USA

SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4338435	A	19820706	US 1981-268944	19810601 <--

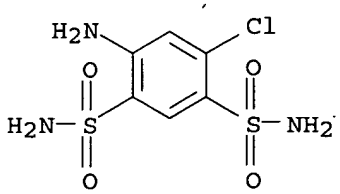
PRIORITY APPLN. INFO.: US 1981-268944 19810601
OTHER SOURCE(S): CASREACT 97:182465
GI



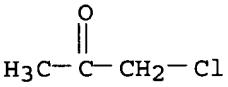
I

AB [(Acylthio)alkyl]benzo]thiadiazine dioxides I (R = H, alkyl, PhCH2; R1 = H, alkyl, Ph; R2, R3, R4, R5, R6, R7, R8, R9, R10, R11 = H, halo, alkyl, Ph; R12 = alkyl, Ph, PhCH2; R13, R14 = H, halo, CF3, SO2NH2, NO2, alkyl, alkoxy; n, m, p, r, s = 0, 1; R1R12 = CH2, CH2CH2) were prepared and are useful as diuretics (no data). Thus, refluxing 5,2,4-Cl(H2NSO2)2C6H2NH2 with AcSCH2CH2CHO in MeCN gave I (n = m = 1, p = r = s = 0, R12 = Me, R13 = 6-Cl, R14 = 7-SO2NH2, R-R5 = H).

IT **121-30-2**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(cyclocondensation of, with β-(acetylthio)propionaldehyde)
RN 121-30-2 HCAPLUS
CN 1,3-Benzenedisulfonamide, 4-amino-6-chloro- (9CI) (CA INDEX NAME)



IT **78-95-5**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(esterification by, of thioacetic acid)
RN 78-95-5 HCAPLUS
CN 2-Propanone, 1-chloro- (8CI, 9CI) (CA INDEX NAME)

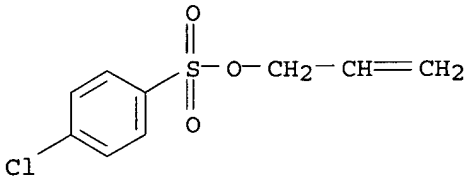


L47 ANSWER 21 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:180349 HCAPLUS
DOCUMENT NUMBER: 96:180349
TITLE: Alkyl and alkenyl esters of sulfonic acids. XXI. Kinetic isotope effects of alkyl and alkenyl esters of sulfonic acid
AUTHOR(S): Sendega, R.; Gorbatenko, N.; Vizgert, R.
CORPORATE SOURCE: Odessa Polytech. Inst., Odessa, USSR
SOURCE: Organic Reactivity (Tartu) (**1980**), 17(3), 247-66
CODEN: ORREDZ; ISSN: 0131-8314
DOCUMENT TYPE: Journal
LANGUAGE: English

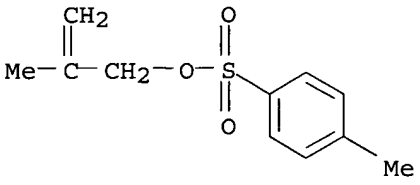
AB The hydrolysis kinetics of p-MeC6H4SO3Cr2CH:CH2, labeled with 14C or α-deuterated, and of different alkyl and alkenyl sulfonates in H2O or D2O are compared with those of alkenyl chlorides and show that the differences in transition states are related to the differences in the degree of covalency of the breaking substrate bond. The transition state structure also depends on the sp. solvation power of the solvent. The occurrence of ion pairing and ion separation in the hydrolyses is discussed.

IT **6165-74-8 20443-62-3 33420-10-9**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(hydrolysis of, solvent isotope effect in relation to kinetics and mechanism of)

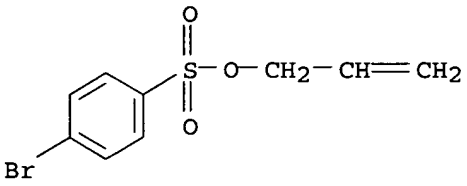
RN 6165-74-8 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-propenyl ester (9CI) (CA INDEX NAME)



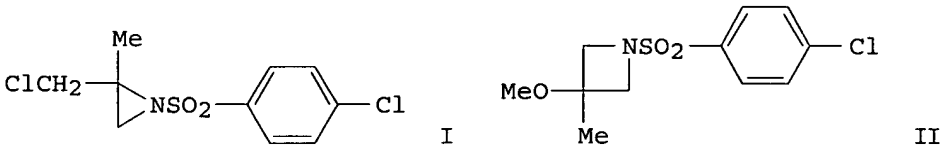
RN 20443-62-3 HCAPLUS
CN 2-Propen-1-ol, 2-methyl-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)



RN 33420-10-9 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-propenyl ester (9CI) (CA INDEX NAME)

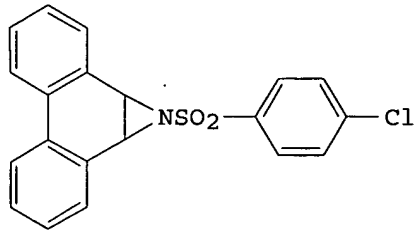


L47 ANSWER 22 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:142585 HCAPLUS
DOCUMENT NUMBER: 96:142585
TITLE: Synthesis and reactions of substituted 1-(arenesulfonyl)aziridines and azetidines
AUTHOR(S): Markov, V. I.; Danileiko, D. A.; Doroshenko, V. A.; Gella, I. M.; Polyakov, A. E.
CORPORATE SOURCE: Dnepropetr. Khim.-Tekhnol. Inst., Dnepropetrovsk, USSR
SOURCE: Org. Soedin. Sery (**1980**), Volume 2, 176-84.
Editor(s): Gal'pern, G. D. Zinatne: Riga, USSR.
CODEN: 38CKA3
DOCUMENT TYPE: Conference
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 96:142585
GI



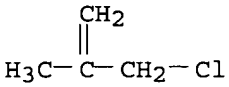
I

II



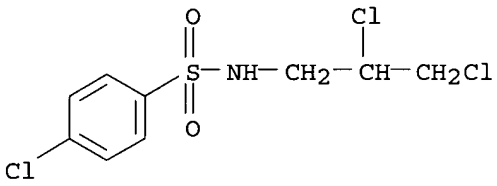
III

AB Addition reaction of 4-ClC6H4SO2NCl2 and CH2:CMeCH2Cl gave 4-ClC6H4SO2NClCH2CMeClCH2Cl, which was N-dichlorinated with Na2SO3, then cyclized to I with aqueous NaOH. I with H2SO4 in MeOH gave 4-ClC6H4SO2NHCH2C(OMe)MeCH2Cl, which with NaOEt gave 14.5% II. Also prepared were several other aziridines, III, and its 9,10-anthracene analog.
IT **563-47-3**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(addition reaction of, with trichlorobenzenesulfonamide)
RN 563-47-3 HCAPLUS
CN 1-Propene, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)

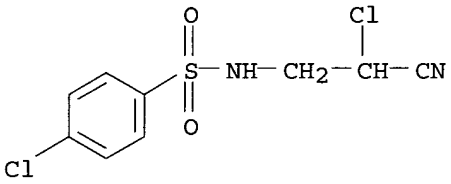


IT **834-70-8P 17260-63-8P 38388-71-5P**
38388-76-0P 38388-82-8P 78050-50-7P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkaline cyclization of)

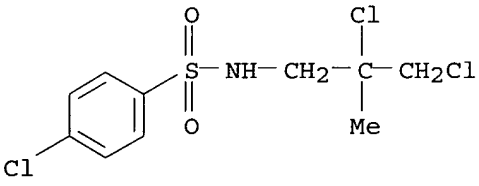
RN 834-70-8 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(2,3-dichloropropyl)- (9CI) (CA INDEX NAME)



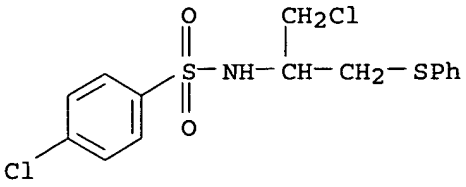
RN 17260-63-8 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(2-chloro-2-cyanoethyl)- (9CI) (CA INDEX NAME)



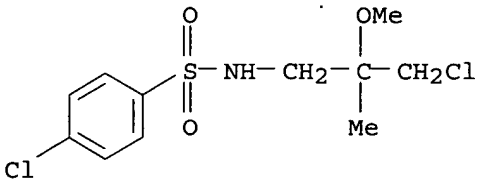
RN 38388-71-5 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(2,3-dichloro-2-methylpropyl)- (9CI) (CA INDEX NAME)



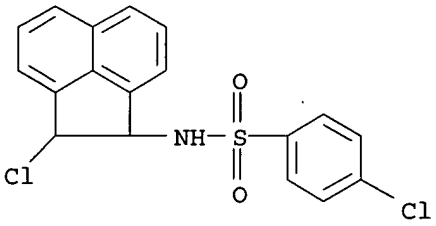
RN 38388-76-0 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-[1-(chloromethyl)-2-(phenylthio)ethyl]- (9CI) (CA INDEX NAME)



RN 38388-82-8 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(3-chloro-2-methoxy-2-methylpropyl)- (9CI) (CA INDEX NAME)



RN 78050-50-7 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(2-chloro-1,2-dihydro-1-acenaphthylenyl)- (9CI) (CA INDEX NAME)



L47 ANSWER 23 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:51998 HCAPLUS
DOCUMENT NUMBER: 96:51998
TITLE: Sulfonic esters of keto alcohols and medicine containing these substances
INVENTOR(S): Fujii, Setsuro; Hamakawa, Toshihiro; Ogawa, Kazuo; Muranaka, Yoshiyuki; Hashimoto, Sadao
PATENT ASSIGNEE(S): Taiho Yakuhin Kogyo K. K., Japan
SOURCE: Fr. Demande, 64 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2475041	A1	19810807	FR 1981-1712	19810129 <--
FR 2475041	B1	19841228		
JP 56108758	A2	19810828	JP 1980-11214	19800131 <--

JP 60059904	B4	19851227		
JP 57021321	A2	19820204	JP 1980-95299	19800711 <--
JP 61030645	B4	19860715		
JP 57059854	A2	19820410	JP 1980-137026	19800930 <--
JP 62053511	B4	19871110		
JP 57102858	A2	19820626	JP 1980-180852	19801219 <--
JP 63018940	B4	19880420		
US 4411911	A	19831025	US 1981-225979	19810119 <--
GB 2068371	A	19810812	GB 1981-1888	19810122 <--
AU 8166677	A1	19810806	AU 1981-66677	19810128 <--
AU 527933	B2	19830331		
CA 1167046	A1	19840508	CA 1981-369549	19810128 <--
CH 655098	A	19860327	CH 1981-599	19810129 <--
DE 3103144	A1	19811126	DE 1981-3103144	19810130 <--
DE 3103144	C2	19921112		
ES 499527	A1	19820201	ES 1981-499527	19810130 <--
NL 8100494	A	19810901	NL 1981-494	19810202 <--
NL 185343	B	19891016		
NL 185343	C	19900316		
US 4489091	A	19841218	US 1983-492873	19830509 <--

PRIORITY APPLN. INFO.:

JP 1980-11214	A	19800131
JP 1980-95299	A	19800711
JP 1980-137026	A	19800930
JP 1980-180852	A	19801219
US 1981-225979	A3	19810119

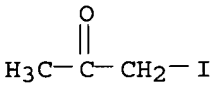
OTHER SOURCE(S): CASREACT 96:51998

AB Sulfonic acids were treated with diazomethyl ketones, and sulfonic acid Ag salts with halomethyl ketones, to yield RSO3CH2CO(CH2)nR1 [R = alkyl, alkoxyalkyl, aralkyl, cycloalkyl, aryl; n = 0-6; R1 = alkyl, alkenyl, halo, OH, alkoxy, carbalkoxy, (alkoxycarbonyl)amino, NHCO2CH2Ph, cycloalkyl, oxacycloalkyl, oxaaryl, aryl], which exhibited anticholesteremic activity. Thus, PhSO3H reacted with PrCOCHN2 in ether to give PhSO3CH2COPr.

IT **3019-04-3**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(esterification of silver benzenesulfonate derivative by)

RN 3019-04-3 HCAPLUS

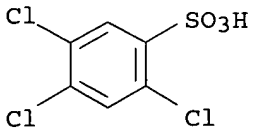
CN 2-Propanone, 1-iodo- (8CI, 9CI) (CA INDEX NAME)



IT **6378-25-2 80524-88-5**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(esterification of, by diazomethyl ketone derivative)

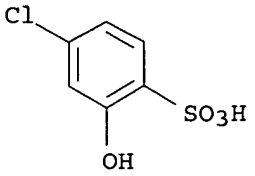
RN 6378-25-2 HCAPLUS

CN Benzenesulfonic acid, 2,4,5-trichloro- (6CI, 7CI, 9CI) (CA INDEX NAME)

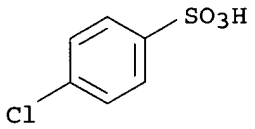


RN 80524-88-5 HCAPLUS

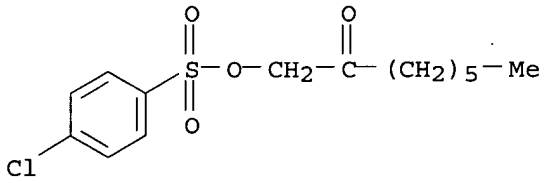
CN Benzenesulfonic acid, 4-chloro-2-hydroxy- (9CI) (CA INDEX NAME)



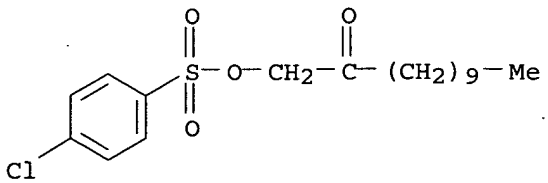
IT **98-66-8**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(esterification of, by diazomethyl ketones)
RN 98-66-8 HCAPLUS
CN Benzenesulfonic acid, 4-chloro- (9CI) (CA INDEX NAME)



IT **80506-30-5P 80506-31-6P 80506-32-7P**
80506-33-8P 80519-87-5P 80520-45-2P
80520-46-3P 80520-47-4P 80520-74-7P
80524-35-2P 80524-39-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and anticholesteremic activity of)
RN 80506-30-5 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-oxooctyl ester (9CI) (CA INDEX NAME)

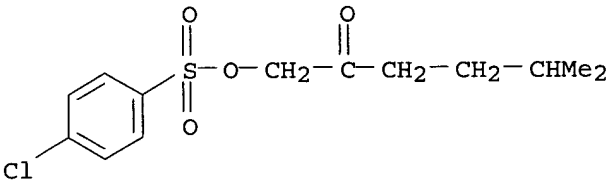


RN 80506-31-6 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-oxododecyl ester (9CI) (CA INDEX NAME)

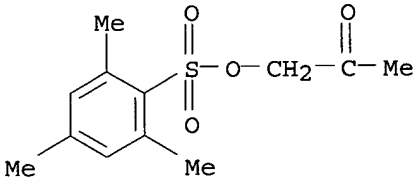


RN 80506-32-7 HCAPLUS

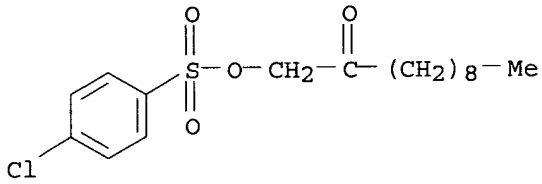
CN Benzenesulfonic acid, 4-chloro-, 5-methyl-2-oxohexyl ester (9CI) (CA INDEX NAME)



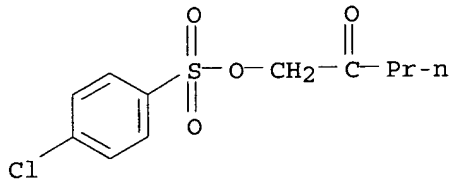
RN 80506-33-8 HCAPLUS
CN Benzenesulfonic acid, 2,4,6-trimethyl-, 2-oxopropyl ester (9CI) (CA INDEX NAME)



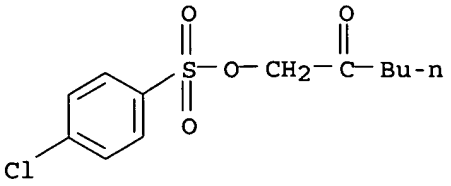
RN 80519-87-5 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-oxoundecyl ester (9CI) (CA INDEX NAME)



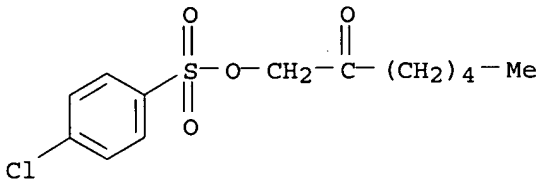
RN 80520-45-2 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-oxopentyl ester (9CI) (CA INDEX NAME)



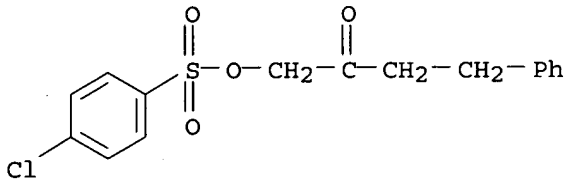
RN 80520-46-3 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-oxohexyl ester (9CI) (CA INDEX NAME)



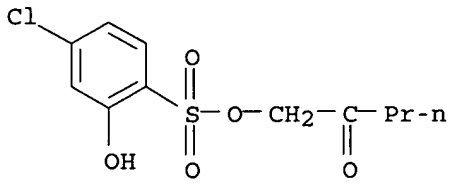
RN 80520-47-4 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-oxoheptyl ester (9CI) (CA INDEX NAME)



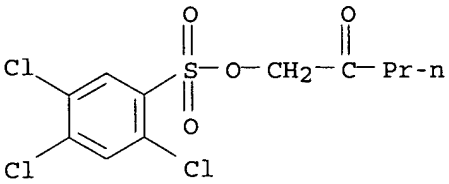
RN 80520-74-7 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-oxo-4-phenylbutyl ester (9CI) (CA INDEX NAME)



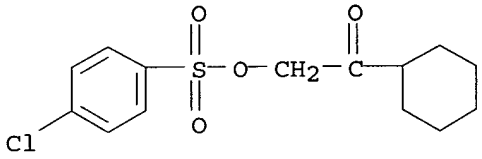
RN 80524-35-2 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-2-hydroxy-, 2-oxopentyl ester (9CI) (CA INDEX NAME)



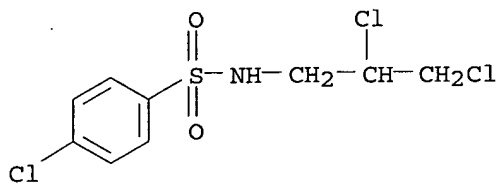
RN 80524-39-6 HCAPLUS
CN Benzenesulfonic acid, 2,4,5-trichloro-, 2-oxopentyl ester (9CI) (CA INDEX NAME)



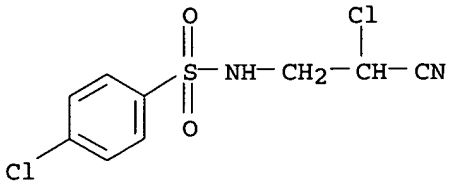
IT **80521-02-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 80521-02-4 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-cyclohexyl-2-oxoethyl ester (9CI) (CA INDEX NAME)



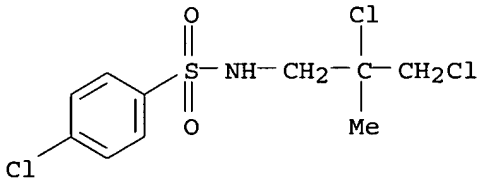
L47 ANSWER 24 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1981:442784 HCAPLUS
DOCUMENT NUMBER: 95:42784
TITLE: Synthesis and reactions of saturated 1-(arenesulfonyl)aziridines and azetidines
AUTHOR(S): Markov, V. I.; Danileiko, D. A.; Doroshenko, V. A.; Gella, I. M.; Polyakov, A. E.
CORPORATE SOURCE: USSR
SOURCE: Organ. Soedin. Sery, Riga (**1980**), (2), 176-84
From: Ref. Zh., Khim. 1981, Abstr. No. 3Zh149
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Title only translated.
IT **834-70-8P 17260-63-8P 38388-71-5P 38388-82-8P 78050-50-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 834-70-8 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(2,3-dichloropropyl)- (9CI) (CA INDEX NAME)



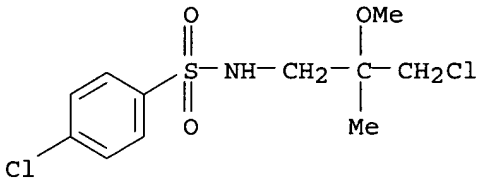
RN 17260-63-8 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(2-chloro-2-cyanoethyl)- (9CI) (CA INDEX NAME)



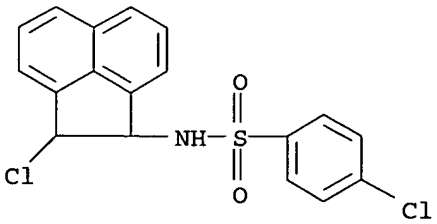
RN 38388-71-5 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(2,3-dichloro-2-methylpropyl)- (9CI) (CA INDEX NAME)



RN 38388-82-8 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(3-chloro-2-methoxy-2-methylpropyl)- (9CI) (CA INDEX NAME)

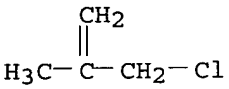


RN 78050-50-7 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(2-chloro-1,2-dihydro-1-acenaphthylenyl)- (9CI) (CA INDEX NAME)

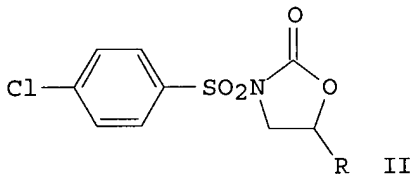


IT **563-47-3**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction of, with dichlorobenzenesulfonamides)

RN 563-47-3 HCAPLUS
CN 1-Propene, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)

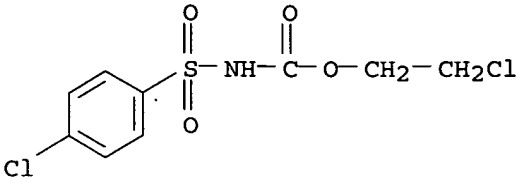


L47 ANSWER 25 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1980:514368 HCAPLUS
DOCUMENT NUMBER: 93:114368
TITLE: Chemistry of sulfonyl isocyanates and sulfonyl isothiocyanates. IX. Routes to substituted oxazolidin-2-ones and oxazolidine-2-thiones
AUTHOR(S): McFarland, J. W.; Hayes, C. E.; Blair, E. B.; Stuhlmacher, K. R.
CORPORATE SOURCE: Dep. Chem., DePauw Univ., Greencastle, IN, 46135, USA
SOURCE: Journal of Heterocyclic Chemistry (**1980**), 17(2), 271-2
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 93:114368
GI

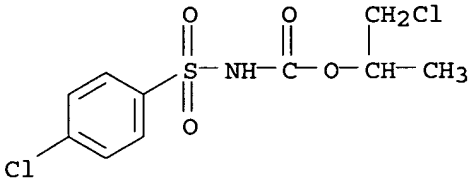


II

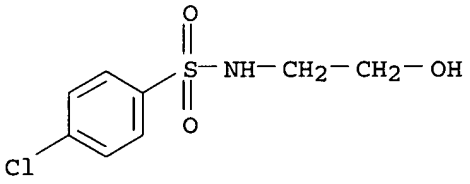
AB p-ClC6H4SO2NCO reacted with 2-chloroethanol and 1-chloro-2-propanol to give p-ClC6H4SO2NHCO2CHRCH2Cl (I; R = H, Me). I cyclized under the influence of pyridine to give the oxazolidinones II. II were stable toward HCl but hydrolyzed in 2 M NaOH solution to p-ClC6H4SO2NHCH2CHROH; p-MeC6H4SO2NCO reacted with 2-chloroethanol to give p-MeC4H4SO2NHC(S)OCH2CH2Cl, which was converted by pyridine to 3-(4-toluenesulfonyl)oxazolidine-2-thione.
IT **63924-75-4P 74668-36-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 63924-75-4 HCAPLUS
CN Carbamic acid, [(4-chlorophenyl)sulfonyl]-, 2-chloroethyl ester (9CI) (CA INDEX NAME)



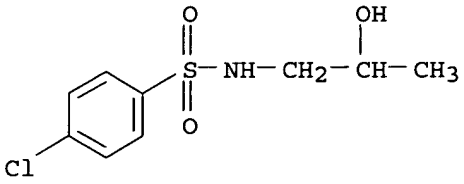
RN 74668-36-3 HCAPLUS
CN Carbamic acid, [(4-chlorophenyl)sulfonyl]-, 2-chloro-1-methylethyl ester (9CI) (CA INDEX NAME)



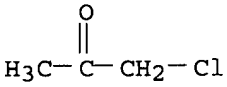
IT **6419-69-8P 74668-38-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 6419-69-8 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



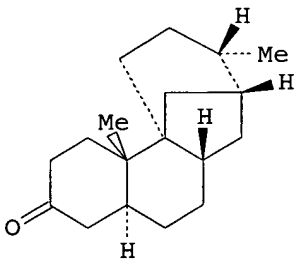
RN 74668-38-5 HCAPLUS
CN Benzenesulfonamide, 4-chloro-N-(2-hydroxypropyl)- (9CI) (CA INDEX NAME)



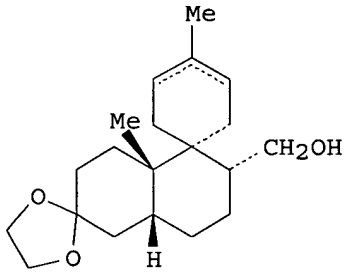
IT **78-95-5**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction of, with chlorobenzenesulfonyl isocyanate)
RN 78-95-5 HCAPLUS
CN 2-Propanone, 1-chloro- (8CI, 9CI) (CA INDEX NAME)



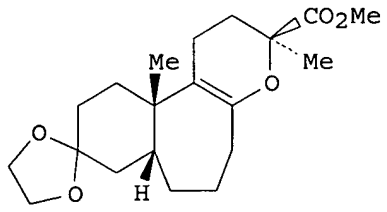
L47 ANSWER 26 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1980:6745 HCAPLUS
DOCUMENT NUMBER: 92:6745
TITLE: Experiments directed toward the total synthesis of terpenes. 24. On the π route to aphidicolin: synthesis of 18,19-bisnoraphidicolan-3-one
AUTHOR(S): Ireland, Robert E.; Aristoff, Paul A.
CORPORATE SOURCE: Chem. Lab., California Inst. Technol., Pasadena, CA, 91125, USA
SOURCE: Journal of Organic Chemistry (**1979**), 44(24), 4323-31
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II



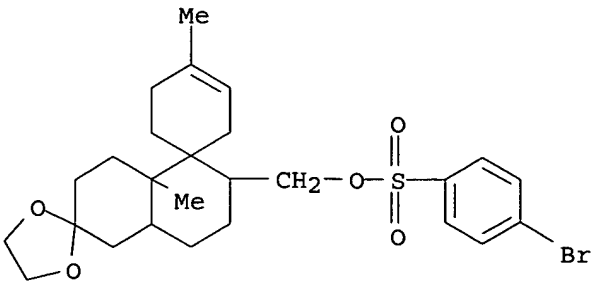
III

AB Aphidicolane-type diterpenes, e.g., I, were prepared by construction of the bicyclo[3.2.1] ring from the tricyclic olefin II. The latter system required the development of spiroketone synthesis which gave III, whose 7-membered ring was contracted via photolysis of a diazoketone.

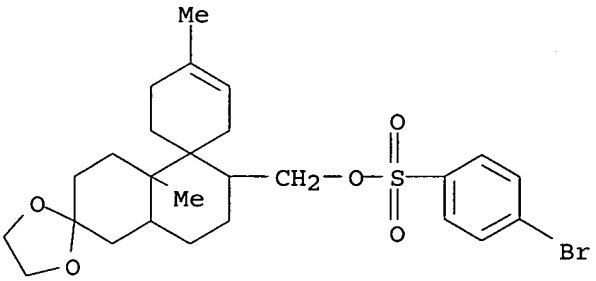
IT **71749-48-9P 71773-11-0P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclodehydration of)

RN 71749-48-9 HCAPLUS

CN Benzenesulfonic acid, 4-bromo-, (3',4',4'a,7',8',8'a-hexahydro-4,8'a-dimethyldispiro[3-cyclohexene-1,1'(2'H)-naphthalene-6'(5'H),2''-[1,3]dioxolan]-2'-yl)methyl ester, (1'α,2'β,4'aα,8'a.alph a.)- (9CI) (CA INDEX NAME)

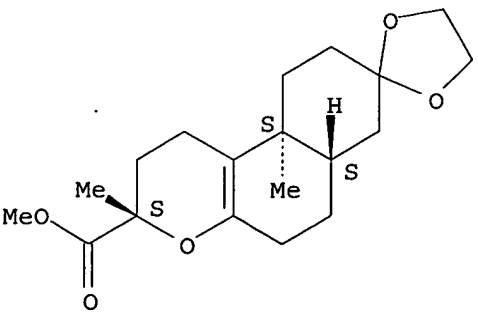


RN 71773-11-0 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, (3',4',4'a,7',8',8'a-hexahydro-4,8'a-dimethyldispiro[3-cyclohexene-1,1'(2'H)-naphthalene-6'(5'H),2''-[1,3]dioxolan]-2'-yl)methyl ester, (1'α,2'α,4'aβ,8'a.beta.)- (9CI) (CA INDEX NAME)



IT **61570-25-0P 61616-09-9P 71749-30-9P**
71773-04-1P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 61570-25-0 HCAPLUS
CN Spiro[1,3-dioxolane-2,8'(6'H)-[1H]naphtho[2,1-b]pyran]-3'-carboxylic acid, 2',3',5',6'a,7',9',10',10'a-octahydro-3',10'a-dimethyl-, methyl ester, (3'α,6'aβ,10'aα)- (9CI) (CA INDEX NAME)

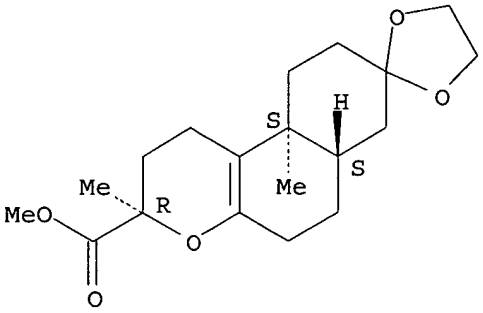
Relative stereochemistry.



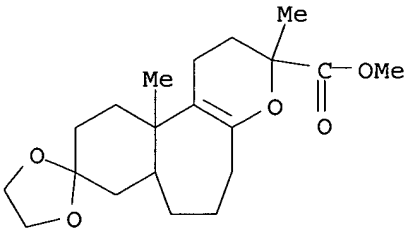
RN 61616-09-9 HCAPLUS
CN Spiro[1,3-dioxolane-2,8'(6'H)-[1H]naphtho[2,1-b]pyran]-3'-carboxylic acid,

2',3',5',6'a,7',9',10',10'a-octahydro-3',10'a-dimethyl-, methyl ester, (3'α,6'aα,10'aβ)- (9CI) (CA INDEX NAME)

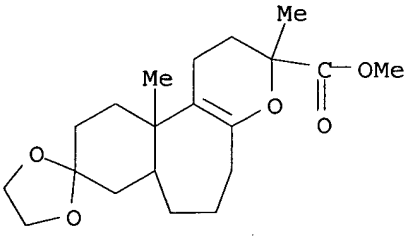
Relative stereochemistry.



RN 71749-30-9 HCAPLUS
CN Spiro[benzo[3,4]cyclohepta[1,2-b]pyran-9(1H),2'-[1,3]dioxolane]-3-carboxylic acid, 2,3,5,6,7,7a,8,10,11,11a-decahydro-3,11a-dimethyl-, methyl ester, (3α,7aα,11aα)- (9CI) (CA INDEX NAME)



RN 71773-04-1 HCAPLUS
CN Spiro[benzo[3,4]cyclohepta[1,2-b]pyran-9(1H),2'-[1,3]dioxolane]-3-carboxylic acid, 2,3,5,6,7,7a,8,10,11,11a-decahydro-3,11a-dimethyl-, methyl ester, (3α,7aβ,11aβ)- (9CI) (CA INDEX NAME)



L47 ANSWER 27 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1975:410102 HCAPLUS
DOCUMENT NUMBER: 83:10102
TITLE: Bicyclic lactam compounds
INVENTOR(S): Lattrell, Rudolf; Lohaus, Gerhard
PATENT ASSIGNEE(S): Farbwerke Hoechst A.-G.
SOURCE: Ger. Offen., 52 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent

LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2325770	A1	19741219	DE 1973-2325770	19730521 <--

PRIORITY APPLN. INFO.: DE 1973-2325770 A 19730521

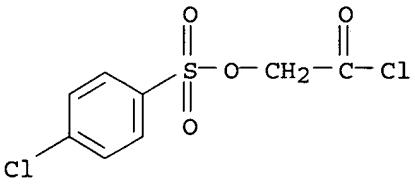
GI For diagram(s), see printed CA Issue.

AB Isomeric cephem derivs: I, II, and III (R = Me, Ph, AcOCH2, EtSCH2CH2, CH2:CH, PhCH2; R1 = Me, Ph; R2 = phthalimido, 4-ClC6H4SO2O, N3, PhCH2CONH) were prepared by cyclodehydration of azetidinones IV with Al or Ti tert-butylate in Me3COH or xylene. (Me3CO)3TiCl, Bu3SnNEt2, TiCl4, MeCaI, AlCl3, and BEt3-diethylboryl pivalate in PhMe and THF were also used. The ratio I-II formed depends on the catalyst and the solvent. II isomerizes to III readily in polar aprotic solvents, whereas this is prevented by the use of tert-alcoholates of Al or Ti. Cis isomers of I show antibacterial activity and the trans isomers are intermediates for pharmaceuticals.

IT **51523-91-2**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(cyclization with propenyl thioformimidate derivative)

RN 51523-91-2 HCAPLUS

CN Benzenesulfonic acid, 4-chloro-, 2-chloro-2-oxoethyl ester (9CI) (CA INDEX NAME)

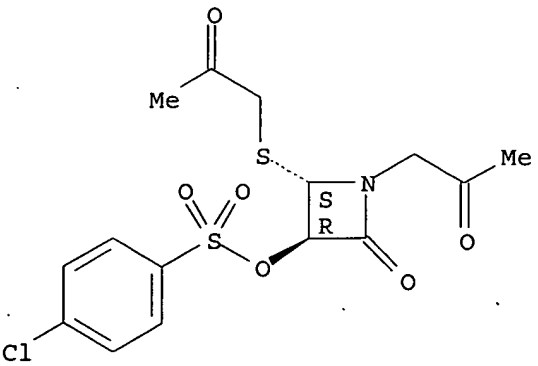


IT **37485-77-1**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(cyclodehydration of)

RN 37485-77-1 HCAPLUS

CN Benzenesulfonic acid, 4-chloro-, 2-oxo-1-(2-oxopropyl)-4-[(2-oxopropyl)thio]-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



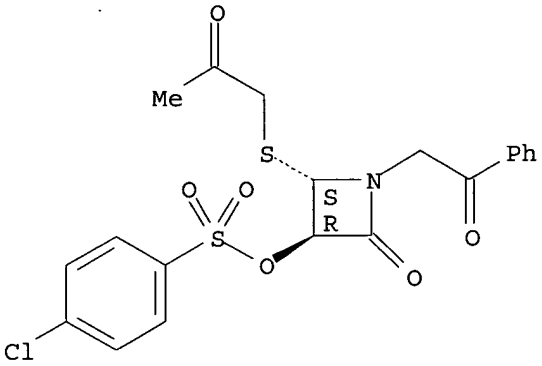
IT **54150-88-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and ketalization and azide exchange)

RN 54150-88-8 HCAPLUS

CN Benzenesulfonic acid, 4-chloro-, 2-oxo-1-(2-oxo-2-phenylethyl)-4-[(2-oxopropyl)thio]-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



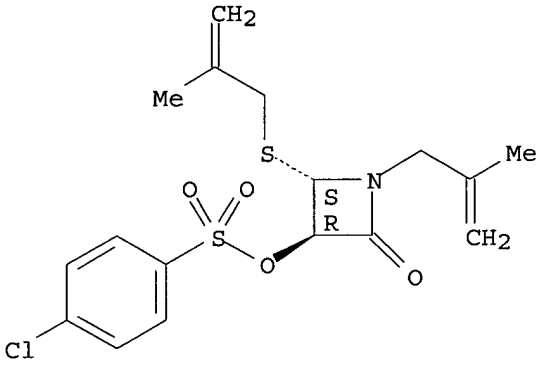
IT **37485-40-8P 54150-17-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and oxidation with ozone)

RN 37485-40-8 HCAPLUS

CN Benzenesulfonic acid, 4-chloro-, 1-(2-methyl-2-propenyl)-2-[(2-methyl-2-propenyl)thio]-4-oxo-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

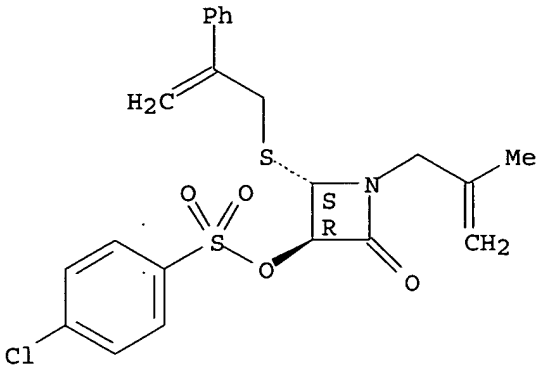
Relative stereochemistry.



RN 54150-17-3 HCAPLUS

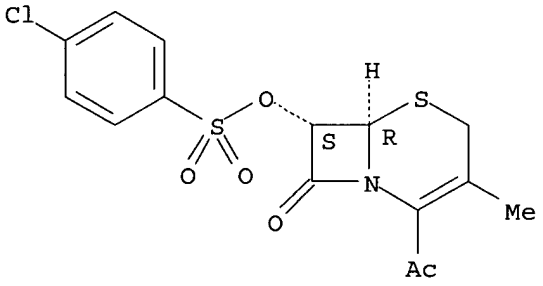
CN Benzenesulfonic acid, 4-chloro-, 1-(2-methyl-2-propenyl)-2-oxo-4-[(2-phenyl-2-propenyl)thio]-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



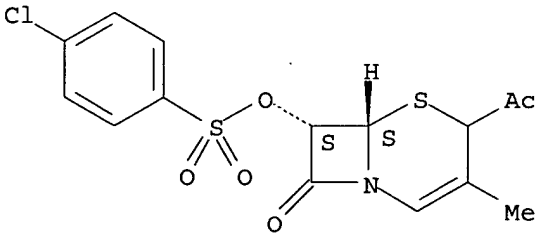
IT **55435-84-2P 55435-85-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 55435-84-2 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-acetyl-3-methyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-7-yl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



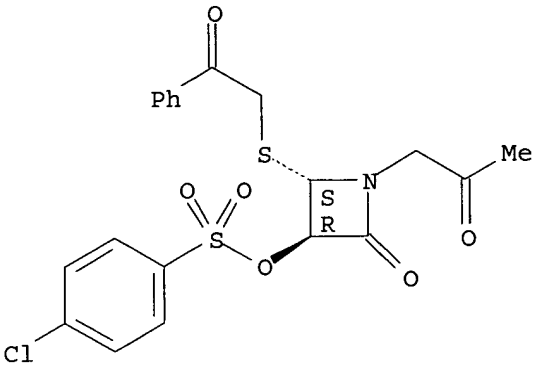
RN 55435-85-3 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 4-acetyl-3-methyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-7-yl ester, (6α,7β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

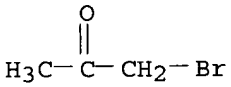


IT **54150-87-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, ketalization, and azido exchange)
RN 54150-87-7 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-oxo-4-[(2-oxo-2-phenylethyl)thio]-1-(2-oxopropyl)-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



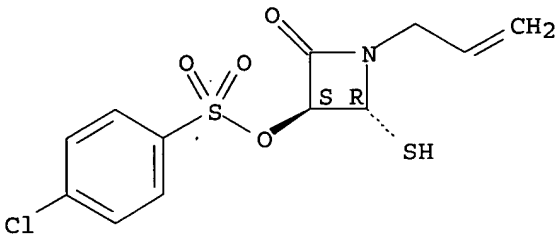
IT **598-31-2**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction of, with diazathiabicycloheptene)
RN 598-31-2 HCAPLUS
CN 2-Propanone, 1-bromo- (8CI, 9CI) (CA INDEX NAME)



L47 ANSWER 28 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1975:4070 HCAPLUS
DOCUMENT NUMBER: 82:4070
TITLE: 4-Mercapto-2-azetidinones. II. Synthesis and reactions of 4-mercapto-2-azetidinones
AUTHOR(S): Lattrell, Rudolf
CORPORATE SOURCE: Hoechst A.-G., Frankfurt/Main, Fed. Rep. Ger.
SOURCE: Justus Liebigs Annalen der Chemie (**1974**), (9), 1361-90
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Reaction of the azetidines I [X = S; R = CPh3; R1 = e.g. CH2COMe, CH2CMe(OMe)2, CH2CO2Me, C(:CMe2)CO2Me, or CH:CPh2; R2 = N3, OAc, phthalimido, NHCOCH2Ph, O3SC6H4Cl-4, or O3SC6H4Me-4] with AgNO3, AcOHgCO2Me, and (AcO)2Hg gave I [X = S, R = Ag] (II), I [X = S, R = HgCO2Me] (III) and the Hg derivs. IV, resp. Treatment of II, III, and IV with H2S gave I (X = S, R = H) (V) as cis and trans isomers. Alkylation of V gave I (X = S; R = CH2COMe, CH2CO2Me, CH2COCH2Ph, CH2COCH2OAc, CH2COCH:CH2, CH2C(:CH2)CO2CMe3, CH2CMe:CH2, or CH2COCH2SEt) which were also prepared by direct alkylation of II, III, or IV. The reaction of V with ClCH2COCH:CH2 and with 2,3-dihydropyran gave no alkylation products but the addition products I (X = S, R = CH2CH2COCH2Cl or 2-tetrahydropyranyl, resp.). The solvolysis of III and IV with excess (AcO)2Hg in MeOH and HOAc, resp., gave I (X = O, R = Me or Ac, resp.). V [R1 = C(:CMe2)CO2Me were investigated regarding their possible occurrence in penicillin chemical
IT **51523-93-4P 51523-95-6P 51524-07-3P**
51585-55-8P 54487-28-4P 54487-34-2P

54487-35-3P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with hydrogen sulfide)
RN 51523-93-4 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-mercapto-4-oxo-1-(2-propenyl)-3-azetidinyl ester, mercury(2+) salt, trans- (9CI) (CA INDEX NAME)

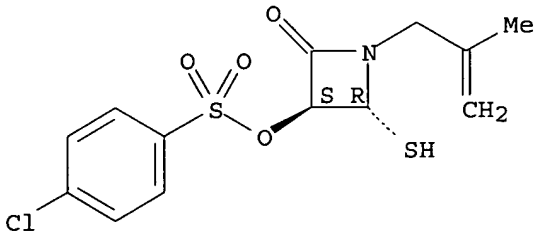
Relative stereochemistry.



●1/2 Hg(II)

RN 51523-95-6 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-mercapto-1-(2-methyl-2-propenyl)-4-oxo-3-azetidinyl ester, mercury(2+) salt, trans- (9CI) (CA INDEX NAME)

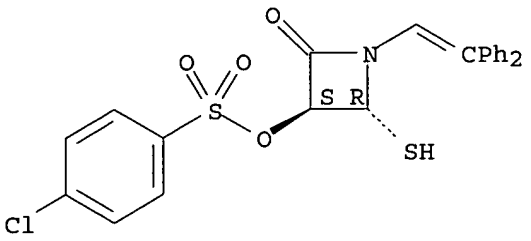
Relative stereochemistry.



●1/2 Hg(II)

RN 51524-07-3 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 1-(2,2-diphenylethenyl)-2-mercapto-4-oxo-3-azetidinyl ester, mercury(2+) salt, trans- (9CI) (CA INDEX NAME)

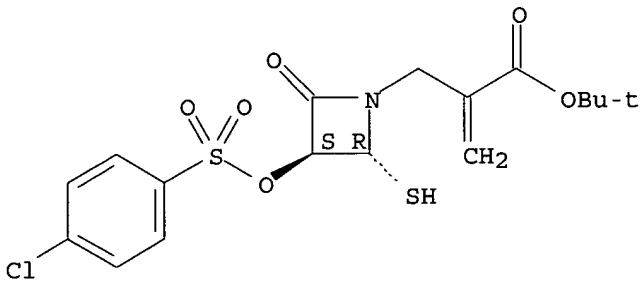
Relative stereochemistry.



●1/2 Hg(II)

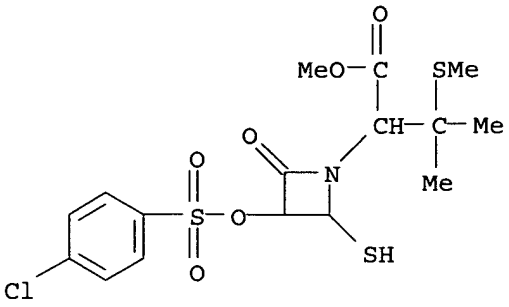
RN 51585-55-8 HCAPLUS
CN 1-Azetidinepropanoic acid, 3-[[(4-chlorophenyl)sulfonyl]oxy]-2-mercapto-α-methylene-4-oxo-, 1,1-dimethylethyl ester, mercury(2+) salt, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



●1/2 Hg(II)

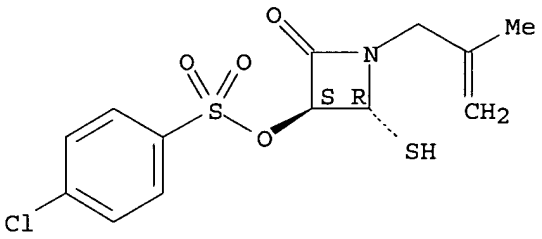
RN 54487-28-4 HCAPLUS
CN 1-Azetidineacetic acid, 3-[[(4-chlorophenyl)sulfonyl]oxy]-2-mercapto-α-[1-methyl-1-(methylthio)ethyl]-4-oxo-, methyl ester, mercury(2+) salt (2:1) (9CI) (CA INDEX NAME)



● 1/2 Hg(II)

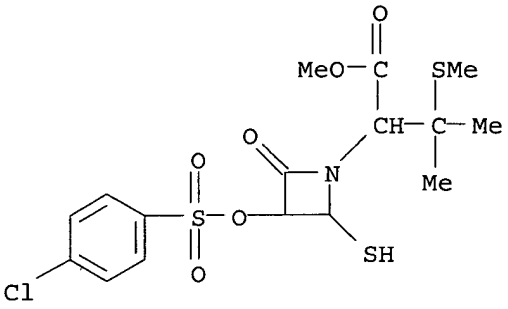
RN 54487-34-2 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-mercapto-1-(2-methyl-2-propenyl)-4-oxo-3-azetidinyl ester, silver(1+) salt, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● Ag(I)

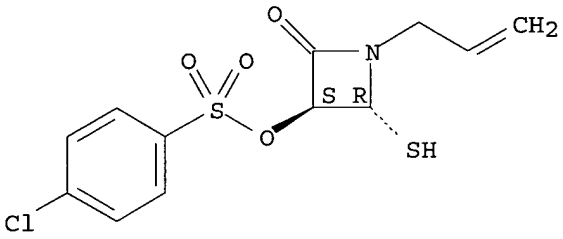
RN 54487-35-3 HCAPLUS
CN 1-Azetidineacetic acid, 4-[[(4-chlorophenyl)sulfonyl]oxy]-2-mercapto-α-[1-methyl-1-(methylthio)ethyl]-4-oxo-, methyl ester, silver(1+) salt (9CI) (CA INDEX NAME)



● Ag(I)

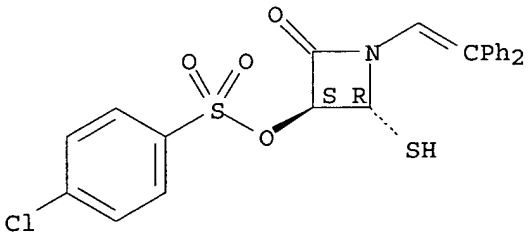
IT **51523-94-5P 51524-08-4P 51750-42-6P**
51887-15-1P 54487-31-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 51523-94-5 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-mercapto-4-oxo-1-(2-propenyl)-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



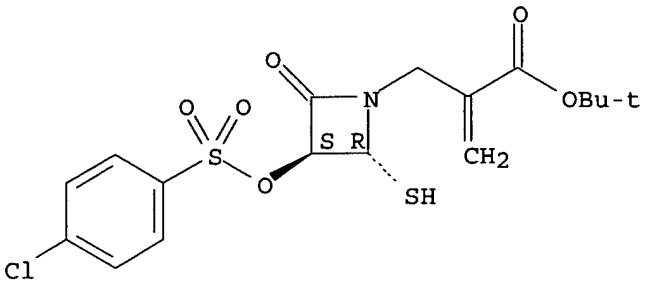
RN 51524-08-4 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 1-(2,2-diphenylethenyl)-2-mercapto-4-oxo-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



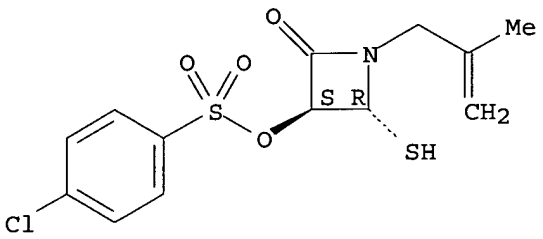
RN 51750-42-6 HCAPLUS
CN 1-Azetidinepropanoic acid, 3-[[(4-chlorophenyl)sulfonyl]oxy]-2-mercapto-α-methylene-4-oxo-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

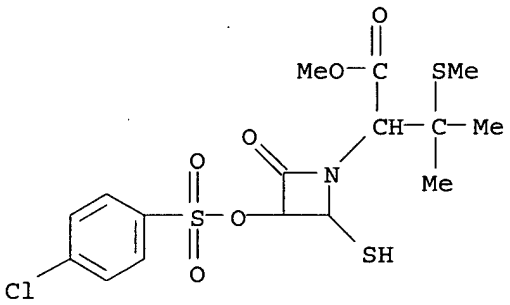


RN 51887-15-1 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-mercapto-1-(2-methyl-2-propenyl)-4-oxo-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

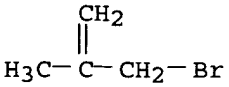
Relative stereochemistry.



RN 54487-31-9 HCAPLUS
CN 1-Azetidineacetic acid, 3-[[(4-chlorophenyl)sulfonyl]oxy]-2-mercapto-α-[1-methyl-1-(methylthio)ethyl]-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

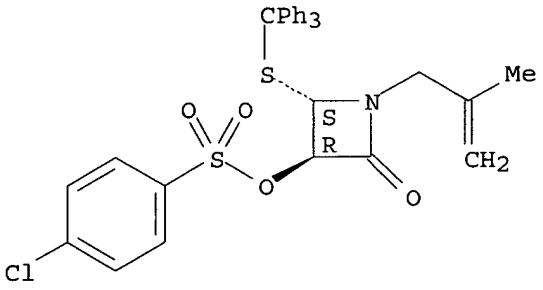


IT **1458-98-6**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction of, with mercaptoazetidinone)
RN 1458-98-6 HCAPLUS
CN 1-Propene, 3-bromo-2-methyl- (9CI) (CA INDEX NAME)



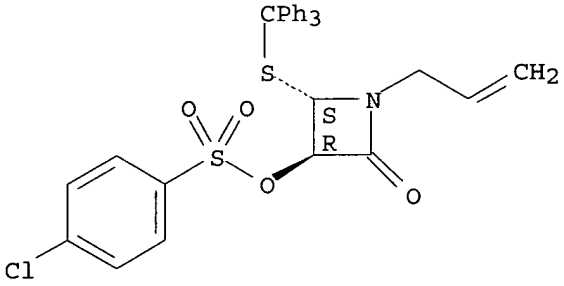
IT **37485-54-4 51523-92-3 51523-99-0**
51524-02-8 51524-06-2
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction of, with mercury salts)
RN 37485-54-4 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 1-(2-methyl-2-propenyl)-2-oxo-4-[(triphenylmethyl)thio]-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



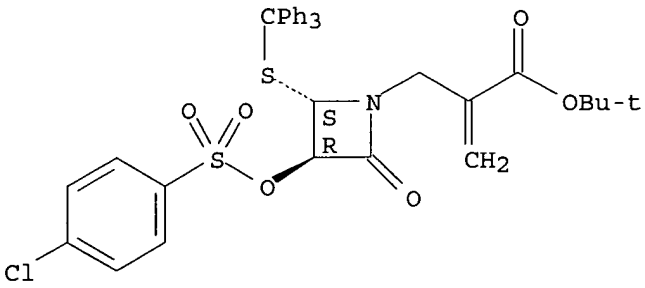
RN 51523-92-3 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-oxo-1-(2-propenyl)-4-[(triphenylmethyl)thio]-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



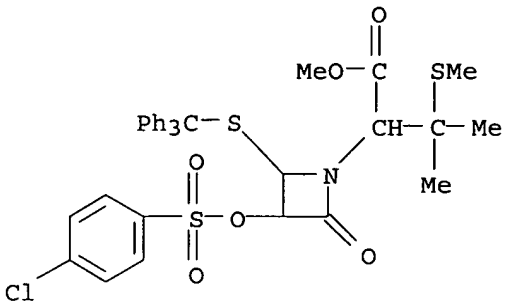
RN 51523-99-0 HCAPLUS
CN 1-Azetidinepropanoic acid, 3-[[(4-chlorophenyl)sulfonyl]oxy]-α-methylene-2-oxo-4-[(triphenylmethyl)thio]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



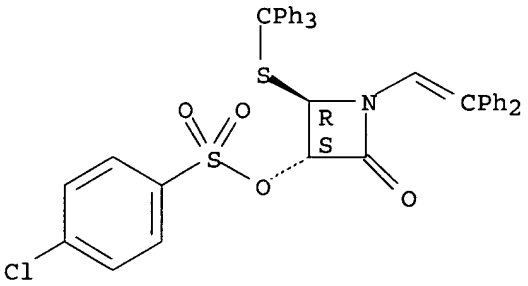
RN 51524-02-8 HCAPLUS

CN 1-Azetidineacetic acid, 3-[[(4-chlorophenyl)sulfonyl]oxy]-α-[1-methyl-1-(methylthio)ethyl]-2-oxo-4-[(triphenylmethyl)thio]-, methyl ester, trans- (9CI) (CA INDEX NAME)



RN 51524-06-2 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 1-(2,2-diphenylethenyl)-2-oxo-4-[(triphenylmethyl)thio]-3-azetidinyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L47 ANSWER 29 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1974:451140 HCAPLUS
DOCUMENT NUMBER: 81:51140
TITLE: Sulfonium salts as dye intermediates
INVENTOR(S): Rempfler, Hermann; Bosshard, Hans; Weber, Kurt
PATENT ASSIGNEE(S): Ciba-Geigy A.-G.
SOURCE: Ger. Offen., 39 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2332709	A1	19740110	DE 1973-2332709	19730627 <--
PRIORITY APPLN. INFO.:			CH 1972-9851 A	19720630

AB Sulfonium salts, used as intermediates for water-insol. salts of anionic dyes, were prepared by reaction of organic halides, alcs., or esters with sulfides. Thus, reaction of (4-ClCH2C6H4)2 with tetrahydrothiophene in 37% aqueous HCl 4 hr at 65.deg. gave 1,1'-(4,4'-biphenylylenedimethylene)bis(tetrahydrothiophenium) dichloride (I) [51382-87-7]. Similarly prepared were 33 other sulfonium salts. I was added to II in H2O to give dye (III) [

51382-86-6], uniform yellow on polyamide 66 fibers.

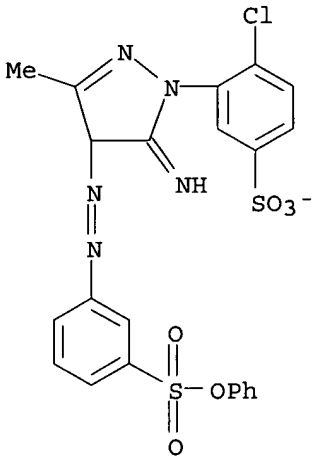
IT **51382-86-6P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)

RN 51382-86-6 HCAPLUS

CN Thiophenium, 1,1'-[[1,1'-biphenyl]-4,4'-diylbis(methylene)]bis[tetrahydro-, salt with 4-chloro-3-[4,5-dihydro-5-imino-3-methyl-4-[[3-(phenoxysulfonyl)phenyl]azo]-1H-pyrazol-1-yl]benzenesulfonic acid (1:2) (9CI) (CA INDEX NAME)

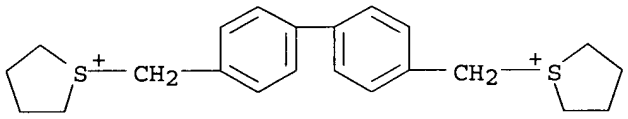
CM 1

CRN 51382-85-5
CMF C22 H17 Cl N5 O6 S2



CM 2

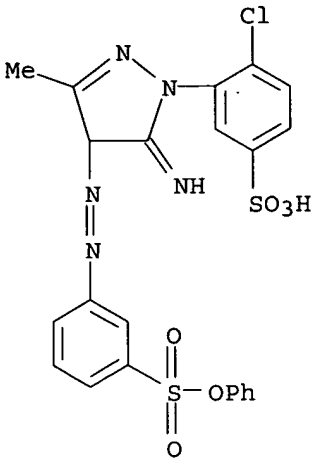
CRN 51382-84-4
CMF C22 H28 S2



IT **52761-33-8**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction of, with (biphenylylenedimethylene)bis(tetrahydrothiophenium) dichloride)

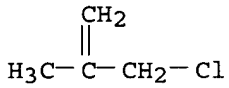
RN 52761-33-8 HCAPLUS

CN Benzenesulfonic acid, 4-chloro-3-[4,5-dihydro-5-imino-3-methyl-4-[[3-(phenoxysulfonyl)phenyl]azo]-1H-pyrazol-1-yl]-, monosodium salt (9CI) (CA INDEX NAME)



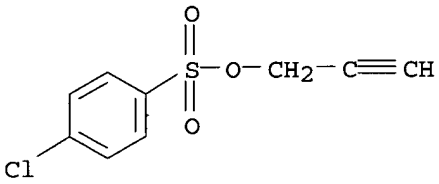
● Na

IT **563-47-3**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction of, with tetrahydrothiophene)
RN 563-47-3 HCAPLUS
CN 1-Propene, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)

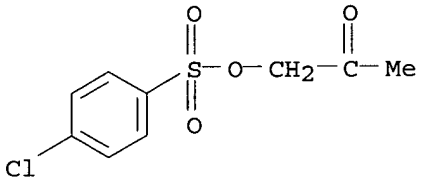


L47 ANSWER 30 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1973:57942 HCAPLUS
DOCUMENT NUMBER: 78:57942
TITLE: Reaction of acetol esters of arenesulfonic acids with substituted phenols
AUTHOR(S): Prib, O. A.; Yasinskii, I. M.
CORPORATE SOURCE: Karagand. Med. Inst., Karaganda, USSR
SOURCE: Zhurnal Organicheskoi Khimii (**1971**), 7(2), 348-50
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB 4-XC6H4SO3CH2COMe (X = H, Cl, Me) (prepared in 65-79% yield by hydrating 4-XC6H4SO3CH2C.tplbond.CH in aqueous MeOH containing H2SO4-HgSO4) reacted with ROH
(R = 2- and 4-BrC6H4, 2- and 4-O2NC6H4) in Me2CO containing K2CO3 at room temperature to give 82.1-92.3% ROCH2COMe. 2,6-Br2C6H3OH and 2,4-Cl2C6H3OH gave the resp. acetol ethers in 53.6 and 58.0% yield, and [5,2-Cl(HO)C6H3]2CH2 afforded the mono- and diethers in 90.1 and 91.2% yield, resp. All of the above products except the dibromophenyl and dichlorophenyl ethers formed semicarbazones in 62-92.0% yield.
IT **6165-77-1**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)

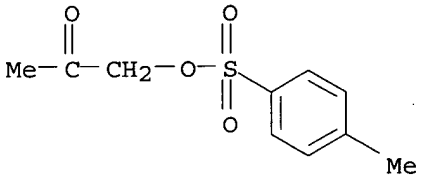
(hydration of)
RN 6165-77-1 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-propynyl ester (9CI) (CA INDEX NAME)



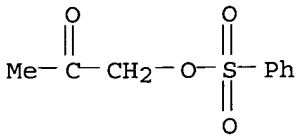
IT **1666-18-8 1666-19-9 1666-20-2**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reaction with phenols)
RN 1666-18-8 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-oxopropyl ester (9CI) (CA INDEX NAME)



RN 1666-19-9 HCAPLUS
CN 2-Propanone, 1-[[(4-methylphenyl)sulfonyl]oxy]- (9CI) (CA INDEX NAME)



RN 1666-20-2 HCAPLUS
CN 2-Propanone, 1-[(phenylsulfonyl)oxy]- (9CI) (CA INDEX NAME)



L47 ANSWER 31 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1971:124637 HCAPLUS
DOCUMENT NUMBER: 74:124637
TITLE: Reactions of unsaturated esters of aromatic sulfonic acids. XV. Solvolysis of 2-methylallyl and

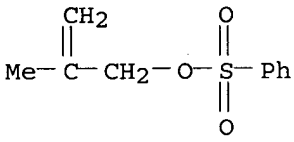
2-methylpropyl esters of substituted benzenesulfonic acid in pure alcohols

AUTHOR(S): Sendega, R. V.; Mikhalevich, M. K.; Vizgert, R. V.
CORPORATE SOURCE: Dep. Gen. Inorg. Chem., Lvov. Polytech. Inst., Lvov, USSR

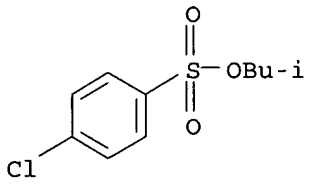
SOURCE: Reaktsionnaya Sposobnost Organicheskikh Soedinenii (1970), 7(3), 636-57
CODEN: RSOTAY; ISSN: 0375-9520
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The kinetics of the solvolysis of 2-methylallyl and 2-methylpropyl esters of substituted benzenesulfonic acid in alcs. ROH (R = Me, Et, n-Pr, n-Bu, iso-Pr, and tert-Bu) was studied at 50, 60, and 70°, and the corresponding activation parameters were calculated Introduction of a Me group into the β-position of a propyl group decreased the solvolysis rate. The magnitude of the substituent effect depended on the magnitude of the pos. charge on the C atom at the reaction center; the less charge the greater the substituent effect. Linear relations of the rate consts. with inductive and steric consts. of the R substituents in the alcs. was observed; the steric effects of R were slight.

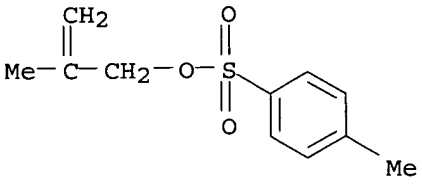
IT **20443-63-4P 32317-63-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20443-63-4 HCAPLUS
CN 2-Propen-1-ol, 2-methyl-, benzenesulfonate (7CI, 8CI, 9CI) (CA INDEX NAME)



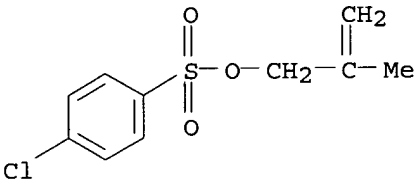
RN 32317-63-8 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



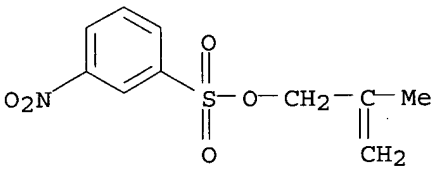
IT **20443-62-3 20443-64-5 20443-65-6**
32317-56-9 32317-58-1 32317-59-2
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(solvolysis of, in alcs.)
RN 20443-62-3 HCAPLUS
CN 2-Propen-1-ol, 2-methyl-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)



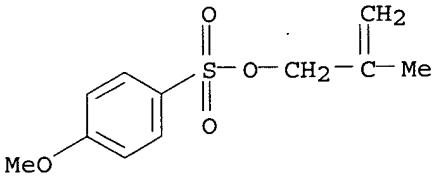
RN 20443-64-5 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-methyl-2-propenyl ester (9CI) (CA INDEX NAME)



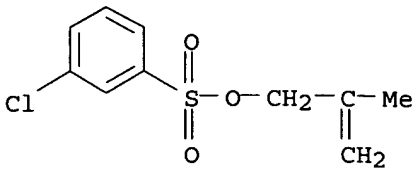
RN 20443-65-6 HCAPLUS
CN Benzenesulfonic acid, 3-nitro-, 2-methyl-2-propenyl ester (9CI) (CA INDEX NAME)



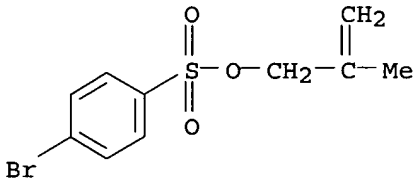
RN 32317-56-9 HCAPLUS
CN Benzenesulfonic acid, 4-methoxy-, 2-methyl-2-propenyl ester (9CI) (CA INDEX NAME)



RN 32317-58-1 HCAPLUS
CN Benzenesulfonic acid, 3-chloro-, 2-methyl-2-propenyl ester (9CI) (CA INDEX NAME)



RN 32317-59-2 HCAPLUS
CN Benzenesulfonic acid, 4-bromo-, 2-methyl-2-propenyl ester (9CI) (CA INDEX NAME)

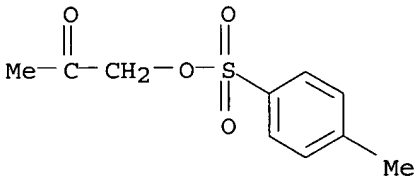


L47 ANSWER 32 OF 32 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:476101 HCAPLUS
DOCUMENT NUMBER: 69:76101
TITLE: Kinetics of the uncatalyzed and alkaline hydrolysis of unsaturated esters of aromatic sulfonic acids
AUTHOR(S): Vizgert, R. V.; Sendega, R. V.
CORPORATE SOURCE: L'vov. Politekh. Inst., Lvov, USSR
SOURCE: Reaktsionnaya Sposobnost Organicheskikh Soedinenii (**1968**), 5(1), 111-26
CODEN: RSOTAY; ISSN: 0375-9520
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Various XC6H4SO3R (I) were prepared by standard methods, the rate consts. of their uncatalyzed hydrolyses in 70% dioxane-water mixts. (k1 in sec.-1) and those of the alkali hydroxide-catalyzed reactions (k2 in l. mole-1 sec.-1) determined, and the energies of activation (E in cal. mole-1), the resp. pre-exponential terms (A), and the entropies of activation [ΔS.++. in cal.(°K.)-1 mole-1] calculated The prepared I were characterized as tabulated. [TABLE OMITTED] The rate consts. were determined spectrophotometrically, conductometrically, and titrimetrically (the spectrophotometric method was the most appropriate). The results are as follows (I, k1 + 105 at 30, 40, and 50°, E, log A, and -ΔS.++. values for the uncatalyzed reaction, k2 + 103 at 30, 40, and 50°, and E, log A, and -ΔS.++. values for the alkaline hydrolysis given): II, 0.0245, 0.0858, 0.278, 23.6, 10.20, 13.36, 0.362,0.991, 2.54, 18.0, 9.54, 15.88; III, 0.0501, 0.142, 0.458, 21.5, 9.21, 18.65, 0.673, 1.99, 3.98, 17.3, 9.31, 17.96; IV, 0.106, 0.355, 1.10,22.7, 10.4, 13.85, 1.595, 3.98, 10.00, 17.8, 10.84, 15.99; V, 0.653,1.735, 4.33, 18.4, 8.09, 23.53, 7.216, 15.85, 41.69, 17.1, 10.20, 13.91;VI, 1.123, 3.37, 9.40, 20.7, 10.07, 15.68, 1.13, 2.72, 6.55, 17.6,9.76, 16.05; VII, 2.250, 6.47, 17.17, 19.8, 9.63, 17.55, 1.76, 4.34,11.06, 17.1, 10.01, 14.74; VIII, 5.62, 15.43, 42.42, 19.6, 10.00,15.30, 4.60, 10.73, 24.60, 16.9, 9.85, 15.49; IX, 27.23, 67.17, 163.0,17.0, 8.70, 20.75, 18.94, 44.80, 98.90, 16.0, 9.80, 15.73; X, 1.45,4.05, 10.60, 19.3, 9.08, 13.82, 1.4730, 4.01, 10.27, 18.9, 10.80, 11.13;XI, 2.49, 7.28, 19.58, 20.1, 9.89, 10.70, 2.369, 5.99, 14.33,

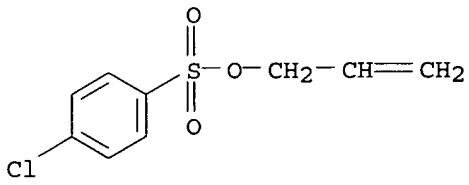
17.5,10.00, 14.80; XII, 7.82, 20.17, 45.62, 18.0, 8.81, 20.26, 6.317,15.00, 35.79, 16.3, 9.57, 17.74; XIII, 39.32, 86.67, 182.2, 14.9,7.34, 26.95, 27.79, 62.80, 134.8, 15.4, 9.54, 16.90; XIV, 13.22(at 0°), 143.5 (at 20°), -, 18.9, 9.76, 15.91, high, high, high,-, -, -; XV, 28.83 (at 0°), 240 (at 20°), -, 16.8,8.59, 23.38, high, high, high, -, -, -; XVI, 8.63, 23.12,46.2, 16.3, 7.70, 20.76, high, high, high, -, -, -; XVII, low, low, low, -, -, -, 2.800, 5.105, 8.09, 10.31, 4.89,38.24; XVIII, -, -, -, -, -, -, 1.815 (at70°), -, 0.291, 20.0, 10.10, 14.93; XIX, -, -, -,-, -, -, 3.210 (at 70°), -, 0.588, 19.1, 9.65, 14.38; XX, -, -, -, -, -, -, 0.210, -, 1.445, 18.8, 9.88, 15.46; and XXI, -, -, -, -, -, -, 0.833, -, 3.450, 18.3, 10.10, 15.28. The σ0 correlation terms for the I reaction series at 30° were evaluated with the following results (R, -log k0, and ρ0 for the uncatalyzed hydrolyses, and -log k0 and ρ0 for the catalyzed reactions given): CH2C.tplbond.CH, 6.30, 1.69, 3.18, 1.53; CH2CH:CH2, 4.65, 1.68, 2.74, 1.46; and CH2CMe:CH2, 4.62, 1.62, 2.60, 1.49. The uncatalyzed hydrolyses are discussed in terms of a 2-step mechanism (the slow 1st step involves the formation of a carbonium ion by splitting the C-O bond.

IT **1666-19-9 6165-74-8 6165-77-1**
20443-62-3 20443-63-4 20443-64-5
20443-65-6 20443-71-4
RL: PEP (Physical, engineering or chemical process); PRP (Properties); **RCT (Reactant)**; PROC (Process); RACT (Reactant or reagent)
(hydrolysis of, kinetics of)

RN 1666-19-9 HCAPLUS
CN 2-Propanone, 1-[[(4-methylphenyl)sulfonyl]oxy]- (9CI) (CA INDEX NAME)



RN 6165-74-8 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-propenyl ester (9CI) (CA INDEX NAME)



RN 6165-77-1 HCAPLUS
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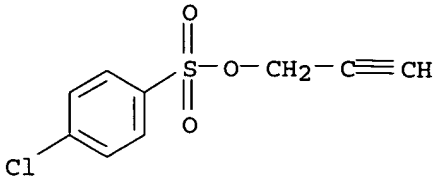
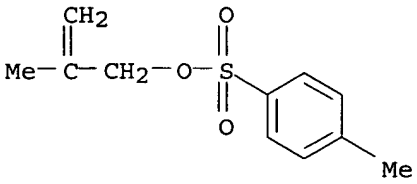


RN 20443-62-3 HCAPLUS
CN 2-Propen-1-ol, 2-methyl-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)



RN 20443-63-4 HCAPLUS
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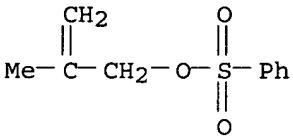
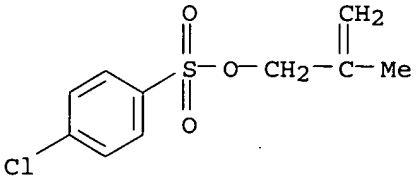
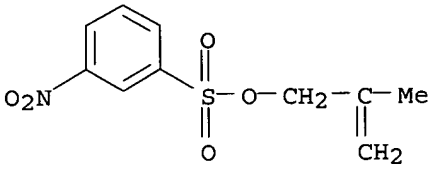


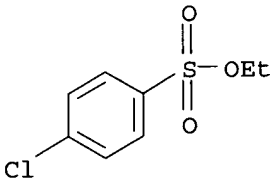
RN 20443-64-5 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, 2-methyl-2-propenyl ester (9CI) (CA INDEX NAME)



RN 20443-65-6 HCAPLUS
CN Benzenesulfonic acid, 3-nitro-, 2-methyl-2-propenyl ester (9CI) (CA INDEX NAME)



RN 20443-71-4 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-, ethyl ester (9CI) (CA INDEX NAME)



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